1-20

Linker can be anything

```
=> d que
L8                  STR
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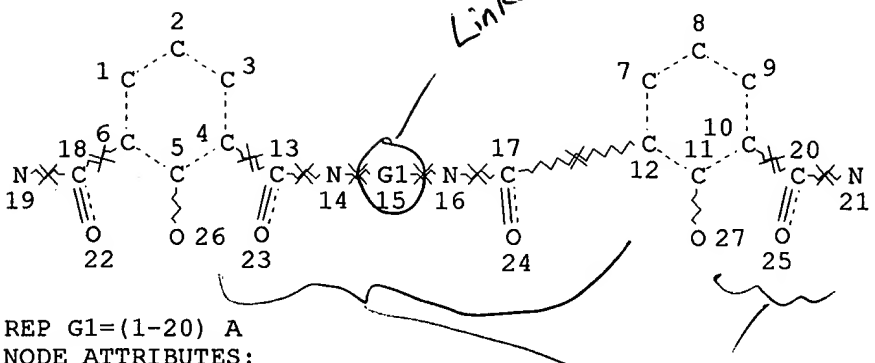

considered 03/20/03 WEC

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DEFAULT ECLEVEL IS LIMITED
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All bonds can be Ring or Chain

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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  27

STEREO ATTRIBUTES: NONE
L15           30 SEA FILE=REGISTRY SSS FUL L8
L16            5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L15


=> d ibib abs hitstr l16 1-5

L16  ANSWER 1 OF 5  HCAPLUS  COPYRIGHT 2003 ACS
ACCESSION NUMBER:         2002:593344 HCAPLUS
DOCUMENT NUMBER:          137:332397
TITLE:                    Figure-of-eight shaped metal-free amide-containing
                          Schiff-base macrocycles and two dicobalt(III) amide
                          complexes
AUTHOR(S):                Brooker, Sally; Dunbar, Geoffrey S.; Weyhermuller,
                          Thomas
CORPORATE SOURCE:         Department of Chemistry, University of Otago, Dunedin,
                          N. Z.
SOURCE:                   Supramolecular Chemistry (2001), 13(5), 601-612
                          CODEN: SCHEER; ISSN: 1061-0278
PUBLISHER:                Gordon & Breach Science Publishers
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
GI
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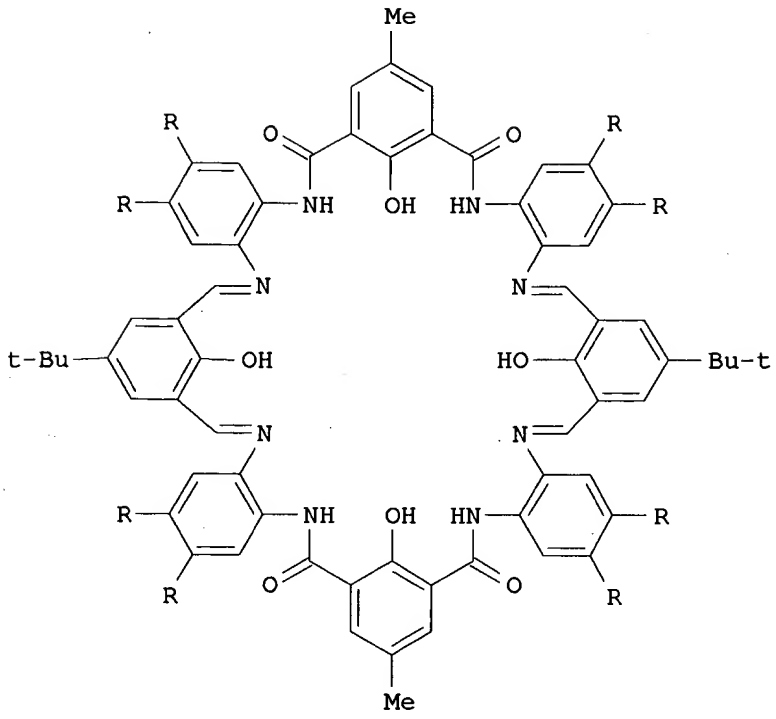


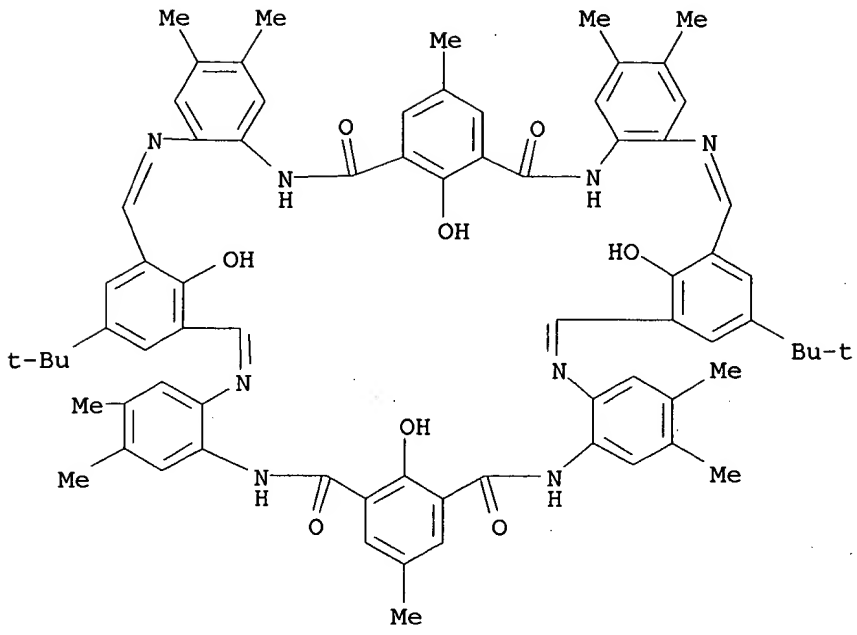
I

AB Two 36-membered (2+2) Schiff-base macrocycles I (R = H, Me) were prepd. and characterized without the use of template ions or high diln. techniques. Rather, intramol. H-bonding and .pi.-.pi. interactions promote the isolation of these figure-of-eight products in good yields. Two Co(III) complexes of the 18-membered (1+1) Schiff-base macrocycles are formed when Co(II) was used as a template. The structures of one figure-of-eight metal-free (2+2) macrocycle and of one dicobalt(III) complex of a (1+1) macrocycle, in which the Co centers are octahedral, are presented. I (R = H), space group P.hivin.1, a 7.747(1), b 17.106(3), c 23.662(4) .ANG., .alpha. 104.83(3), .beta. 95.86(3), .gamma. 97.80(3).degree., U = 2972.4(8) .ANG.3, Z = 2, dc = 1.30 g cm-3, T = 100 K, 554 parameters, R1 = 0.072 for 4137 reflections having F>4[(F)], wR2 = 0.191 and goodness of fit 0.97 (for all 8343 independent F2 data). [Co2I(OAc)2(py)].1.5DMF 0.5MeCN (R = H), space group P2(1)/n, a 13.067(2), b 26.071(4), c 14.023(3) .ANG., .beta. 93.02(1).degree., U = 4770.6(15) .ANG.3, Z = 4, dc = 1.38 g cm-3, T = 168 K, 622 parameters, R1 = 0.075 for 5233 reflections having F>4[(F)], wR2 = 0.133 and goodness of fit 1.08 (for all 8512 independent F2 data).

IT **473705-65-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn.)

RN 473705-65-6 HCAPLUS

CN 7,11:20,24:33,37:46,50-Tetramethenotetrabenz[b,m,x,i1][1,4,12,15,23,26,34,37]octaazacyclotetratetracontine-19,25,45,51(18H,26H,44H,52H)-tetrone, 9,35-bis(1,1-dimethylethyl)-53,54,55,56-tetrahydroxy-2,3,15,16,22,28,29,41,42,48-decamethyl- (9CI) (CA INDEX NAME)



IT **473705-64-5P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure)
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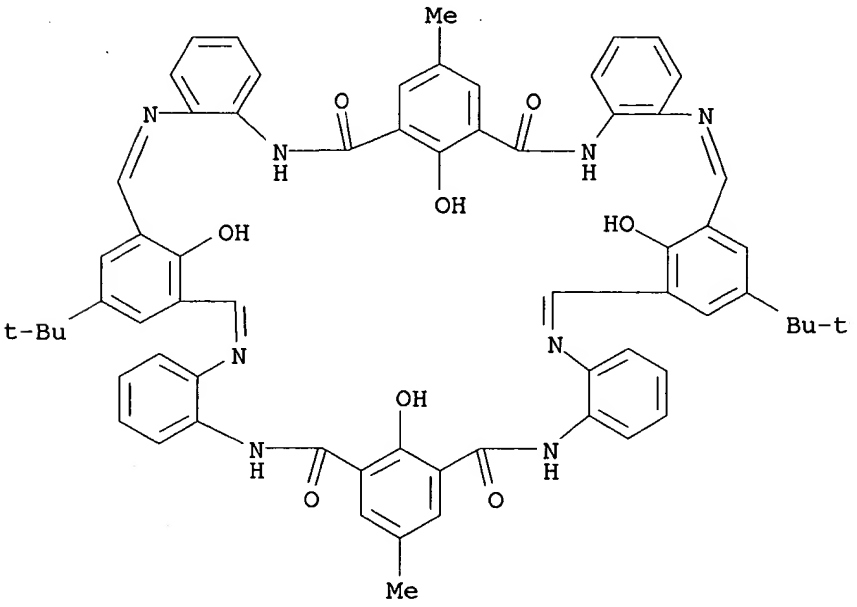
CN 7,11:20,24:33,37:46,50-Tetramethenotetrabenz[b,m,x,i1][1,4,12,15,23,26,34,37]octaazacyclotetratetracontine-6,12,32,38(5H,13H,31H,39H)-tetrone, 22,48-bis(1,1-dimethylethyl)-53,54,55,56-tetrahydroxy-9,35-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:592692 HCAPLUS
DOCUMENT NUMBER: 133:171468
TITLE: Phthalamide-lanthanide complexes for use as luminescent markers
INVENTOR(S): Raymond, Kenneth N.; Petoud, Stephane; Cohen, Seth; Xu, Jide
PATENT ASSIGNEE(S): Regents of the University of California, USA
SOURCE: PCT Int. Appl., 149 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000048990	A1	20000824	WO 2000-US4258	20000218
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1154990	A1	20011121	EP 2000-910246	20000218
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 2002188111	A1	20021212	US 2000-507630	20000218
US 6515113	B2	20030204		
US 2002128451	A1	20020912	US 2001-992156	20011114

PRIORITY APPLN. INFO.:
US 1999-120881P P 19990218
US 1999-120600P P 19990218
US 2000-507630 A3 20000218
WO 2000-US4258 W 20000218

OTHER SOURCE(S): MARPAT 133:171468
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention provides luminescent lanthanide metal chelates comprising a metal ion of the lanthanide series and a macrocyclic complexing agent comprising at least one phthalamidyl moiety. Claimed are the phthalamidyl-contg. ligands, e.g., I [R1, R2, R4, R5, R6, R7, R10, R20 = H, (un)substituted alkyl with proviso for optional presence of rings; R3, R8, R9 = (un)substituted alkyl or aryl; R11, R12, R13, R21, R22, R23 = (un)substituted alkyl, H, various amines, nitro, OH, various alkoxy, etc.; Q1 = OR18 and Q2 = OR19 where R18 and R19 are H, enzymically labile group, hydrolytically labile group, neg. charge; a, z = 0 or 1 with provisos].

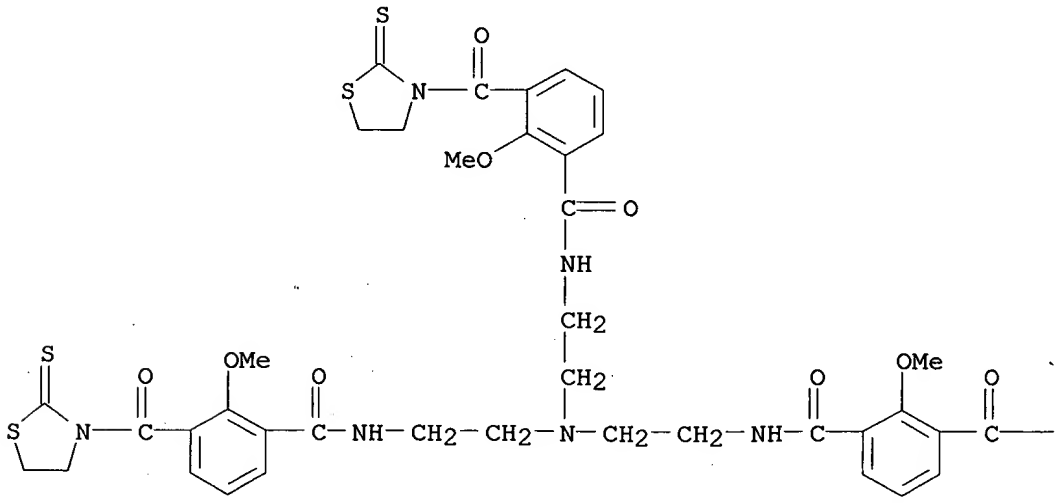
The compds. may incorporate recognition moieties such as polyethers and dendrimers, or are covalently attached to a carrier mol., e.g., small mol. bioactive agents, synthetic polymers and biomols., including antibodies, antigens, peptides, nucleic acids, enzymes, haptens, carbohydrates, and pharmaceutically active agents. The lanthanide metal complexes are luminescent. Also provided are probes incorporating the phthalamidyl ligands of the invention, methods using the ligands of the invention, and probes comprising the ligands of the invention. Provided are methods for detg. whether a sample contains an enzyme, whether a compd. alters an activity of an enzyme, detecting a nucleic acid target sequence, detecting amplification of a target sequence, and ascertaining whether a first nucleic acid and a second nucleic acid hybridize. Also provided are probes incorporating the phthalamidyl ligands of the invention and methods using the ligands of the invention and probes comprising the ligands of the invention. Also claimed is a microarray comprising the lanthanide complex, and said quencher being conjugated directly to a solid support or to a carrier mol. attached to the solid support, and a method for probing the microarray for the presence of a compd. Also provided are use of the complexes for radiation therapy, photodynamic therapy, as a component in an ink or dye, as a component of a substrate for transmission and amplification of light, for performing a fluorescence assay of an analyte, and for selective ion sepn. Thus, the synthesis of bicappedTRENSAM, ligand II, is presented along with the prepn. of its Eu and Tb complexes, both of which are luminescent. Other examples are provided.

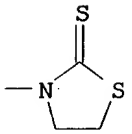
IT **247039-31-2P 247039-38-9P 288099-60-5P**
288099-61-6P 288099-64-9P 288099-67-2P
288099-70-7P 288099-73-0P 288099-74-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for prepn. of phthalamidyl-contg. complexing agent)

RN 247039-31-2 HCAPLUS

CN Benzamide, N,N',N''-(nitrilotri-2,1-ethanediyl)tris[2-methoxy-3-[(2-thioxo-3-thiazolidinyl)carbonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A





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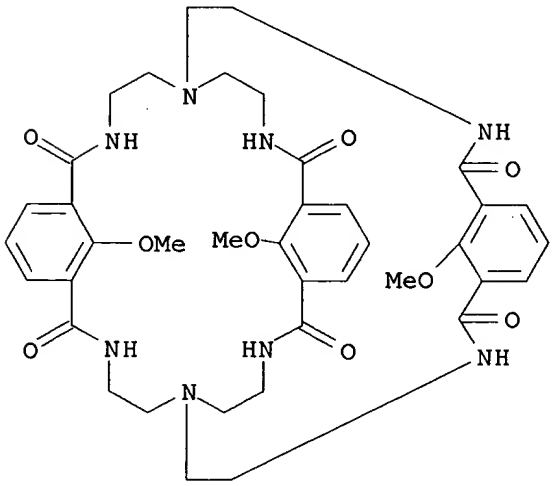
CN 1,4,12,15,18,26,31,39-Octaazapentacyclo[13.13.13.16,10.120,24.133,37]tetra tetraconta-6,8,10(44),20,22,24(43),33,35,37(42)-nonaene-5,11,19,25,32,38-hexone, 42,43,44-trimethoxy- (9CI) (CA INDEX NAME)



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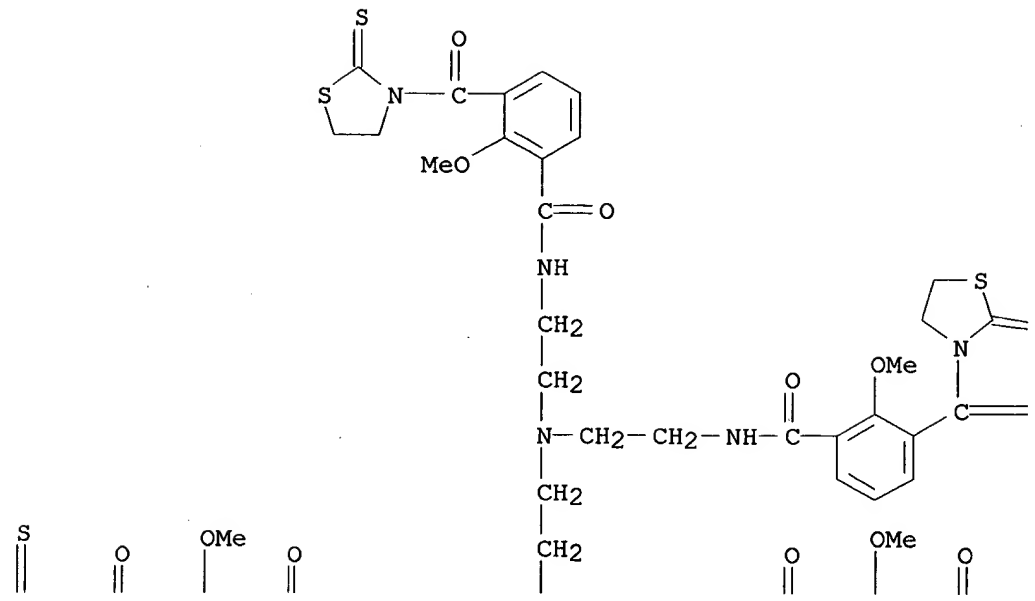
PAGE 1-A



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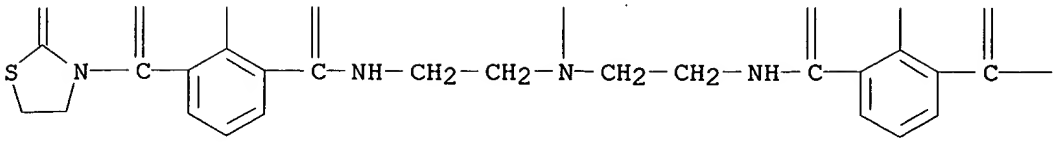
PAGE 2-A



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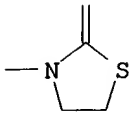

RN 288099-61-6 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'',N'''',N''''''-[1,2-ethanediylbis(nitrilodi-2,1-ethanediyl)]tetrakis[2-methoxy-N'-methyl- (9CI) (CA INDEX NAME)

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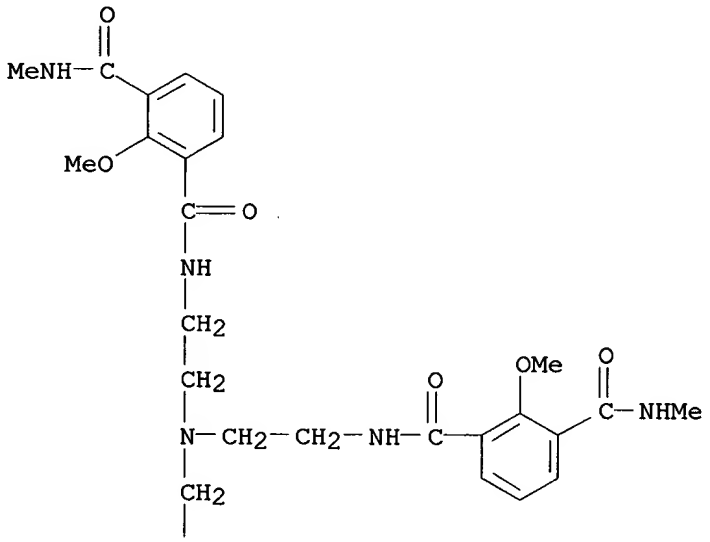

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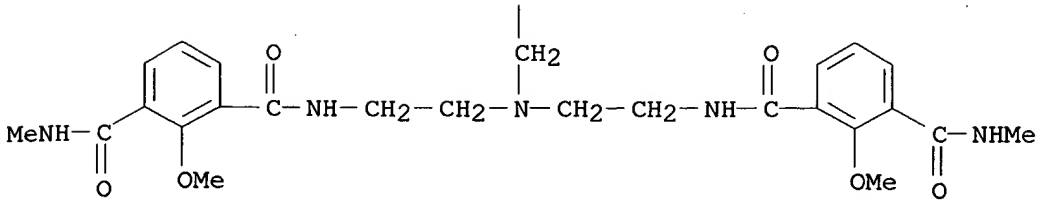
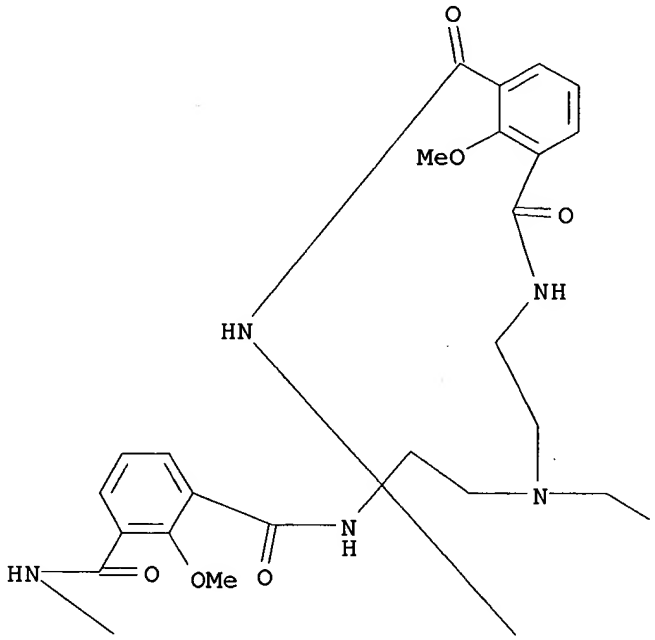


RN 288099-64-9 HCAPLUS
CN 1,4,7,15,18,21,24,32,37,45,52,60-Dodecaazaheptacyclo[19.13.13.134,18.19,13.126,30.139,43.154,58]tetrahexaconta-9,11,13(63),26,28,30(49),39,41,43(48),54,56,58(64)-dodecaene-8,14,26,31,38,44,53,59-octone, 48,49,63,64-tetramethoxy- (9CI) (CA INDEX NAME)

PAGE 1-A



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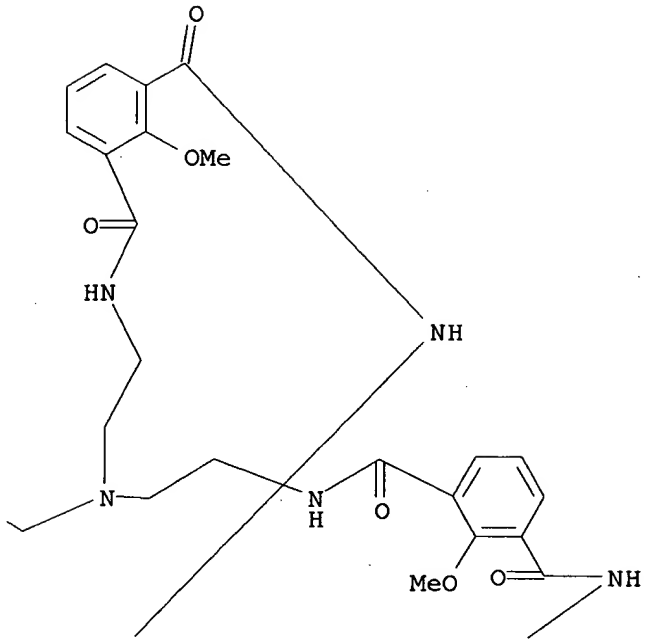

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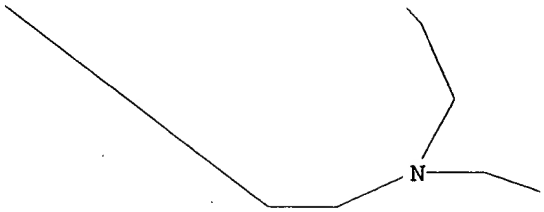

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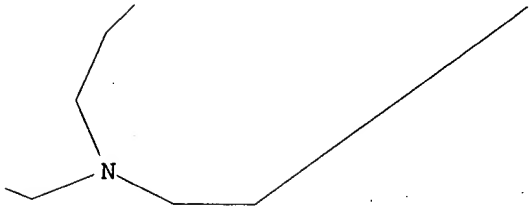
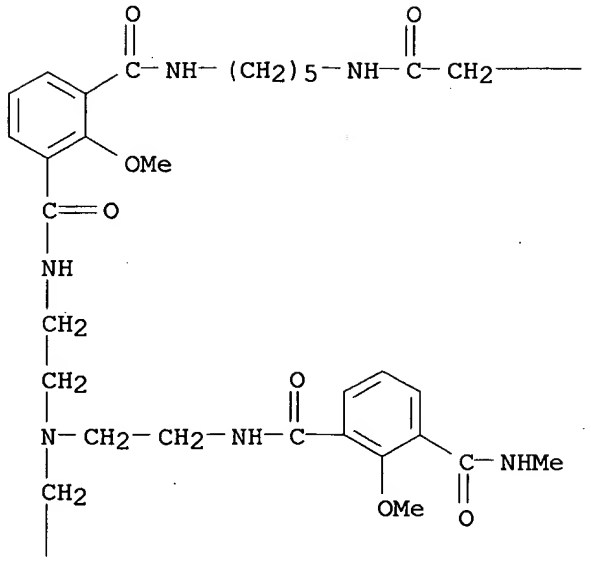


RN 288099-67-2 HCAPLUS
CN Butanoic acid, 4-[[5-[[3-[5,8-bis[2-[[2-methoxy-3-[(methylamino)carbonyl]benzoyl]amino]ethyl]-12-[2-methoxy-3-[(methylamino)carbonyl]phenyl]-1,12-dioxo-2,5,8,11-tetraazadodec-1-yl]-2-methoxybenzoyl]amino]pentyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

PAGE 1-A



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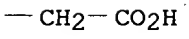

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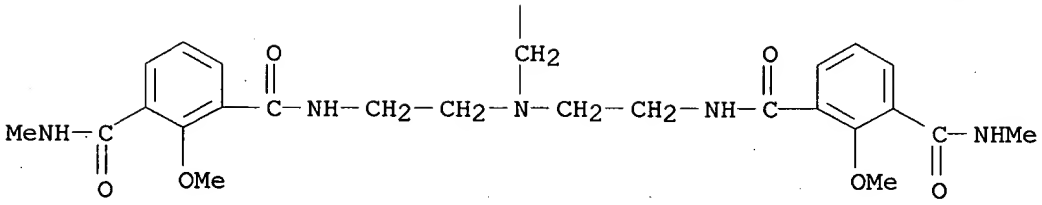
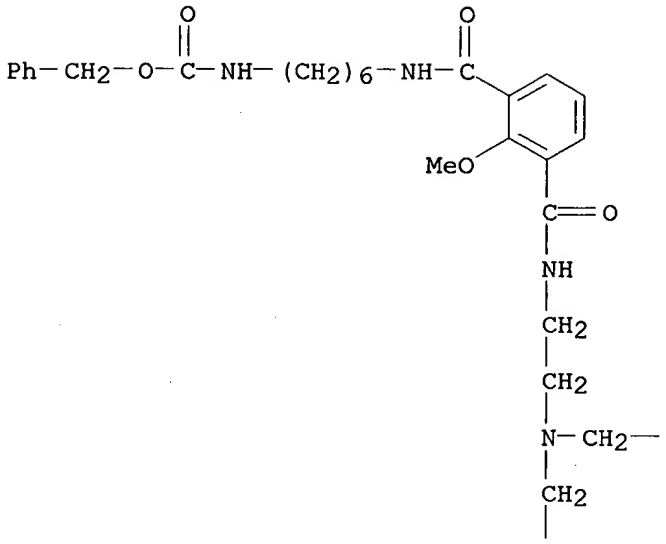


RN 288099-70-7 HCAPLUS
CN Carbamic acid, [1,2-ethanediylbis[nitrilobis[2,1-ethanediyliminocarbonyl(2-methoxy-3,1-phenylene)carbonylimino-6,1-hexanediyl]]]tetrakis-, tetrakis(phenylmethyl) ester (9CI) (CA INDEX NAME)

PAGE 1-A



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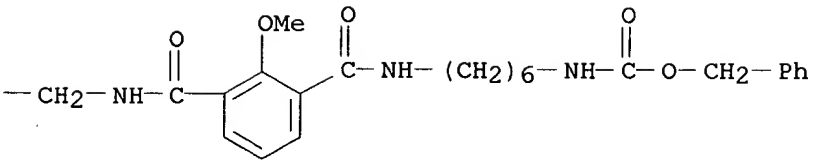

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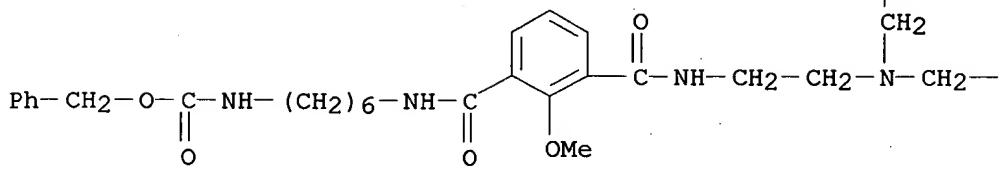

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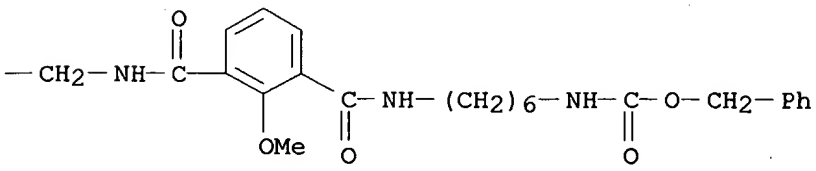

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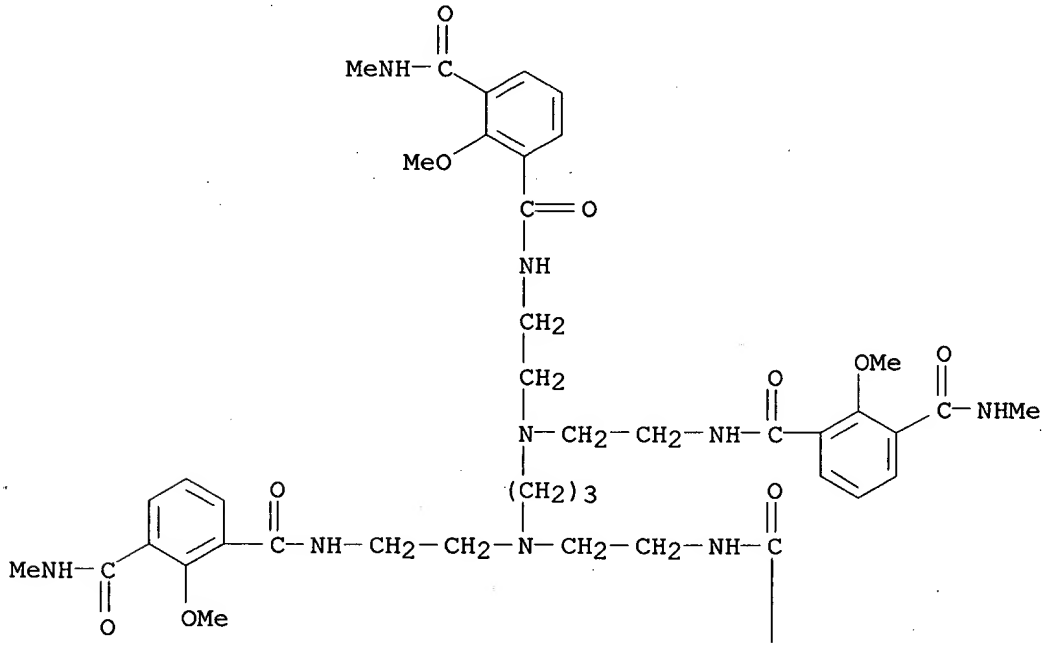
CN 1,3-Benzenedicarboxamide, N,N'',N'''',N''''''-[1,3-propanediylbis(nitrilodi-2,1-ethanediyl)]tetrakis[2-methoxy-N'-methyl-(9CI) (CA INDEX NAME)

PAGE 1-A



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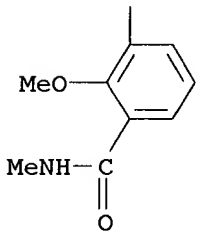

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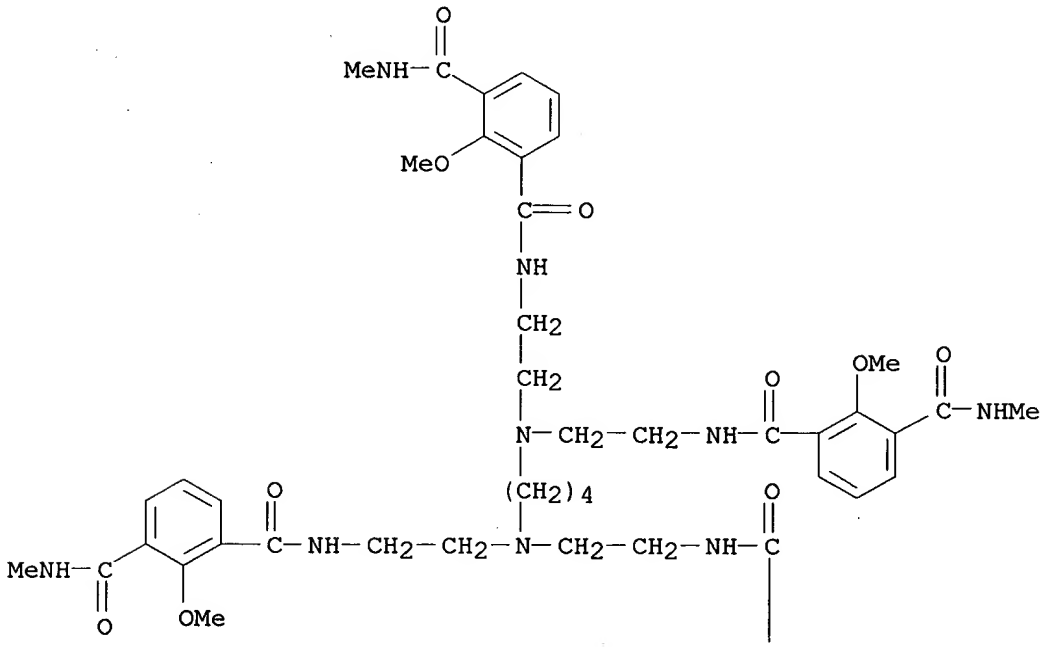
PAGE 1-A



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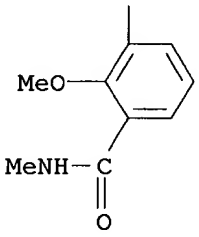
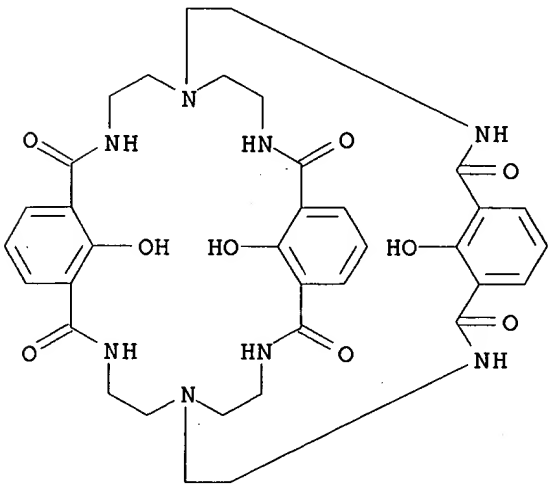


IT **247039-39-0P 288099-66-1P 288099-68-3P**

288099-71-8P 288099-75-2P 288099-76-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and complexation with lanthanide ions)

RN 247039-39-0 HCAPLUS
CN 1,4,12,15,18,26,31,39-Octaazapentacyclo[13.13.13.16,10.120,24.133,37]tetra tetraconta-6,8,10(44),20,22,24(43),33,35,37(42)-nonaene-5,11,19,25,32,38-hexone, 42,43,44-trihydroxy-, dihydrobromide (9CI) (CA INDEX NAME)



●2 HBr

RN 288099-66-1 HCAPLUS
CN 1,4,7,15,18,21,24,32,37,45,52,60-Dodecaazaheptacyclo[19.13.13.134,18.19,13.126,30.139,43.154,58]tetrahexaconta-9,11,13(63),26,28,30(49),39,41,43(48),54,56,58(64)-dodecaene-8,14,26,31,38,44,53,59-octone, 48,49,63,64-tetrahydroxy- (9CI) (CA INDEX NAME)

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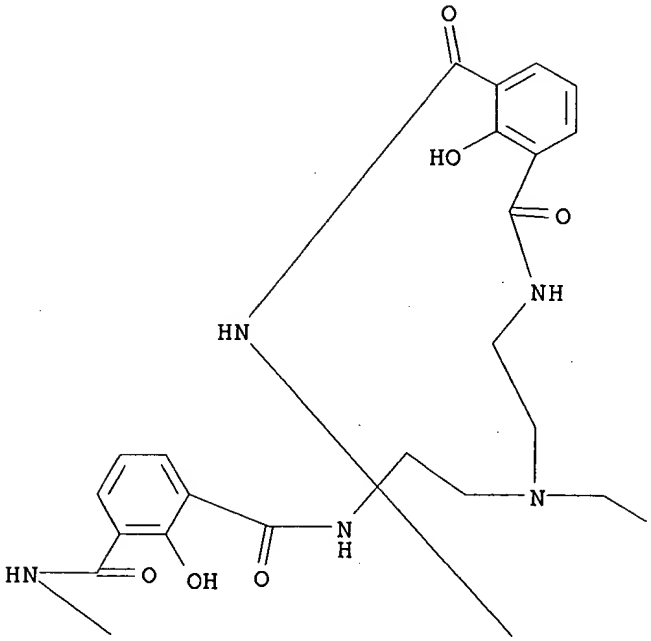

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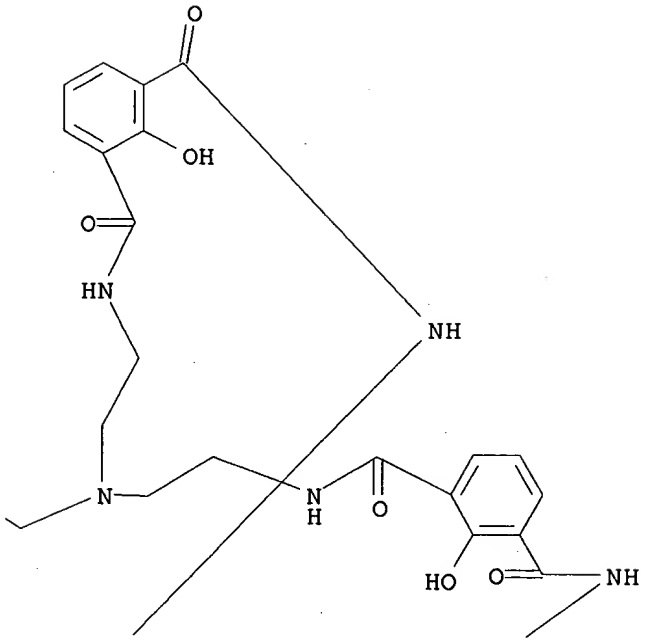

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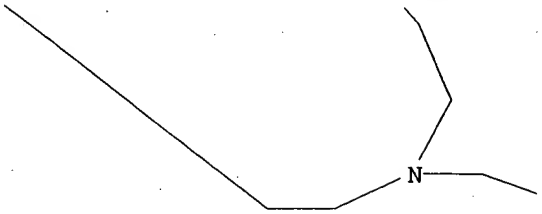

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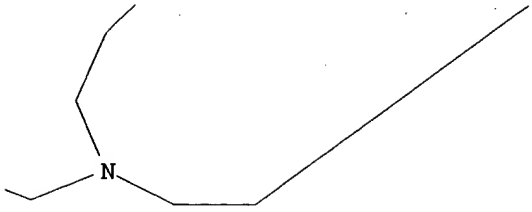

RN 288099-68-3 HCAPLUS
CN Butanoic acid, 4-[[5-[[3-[5,8-bis[2-[[2-hydroxy-3-[(methylamino)carbonyl]benzoyl]amino]ethyl]-12-[2-hydroxy-3-[(methylamino)carbonyl]phenyl]-1,12-dioxo-2,5,8,11-tetraazadodec-1-yl]-2-hydroxybenzoyl]amino]pentyl]amino]-4-oxo-, dihydrobromide (9CI) (CA INDEX NAME)

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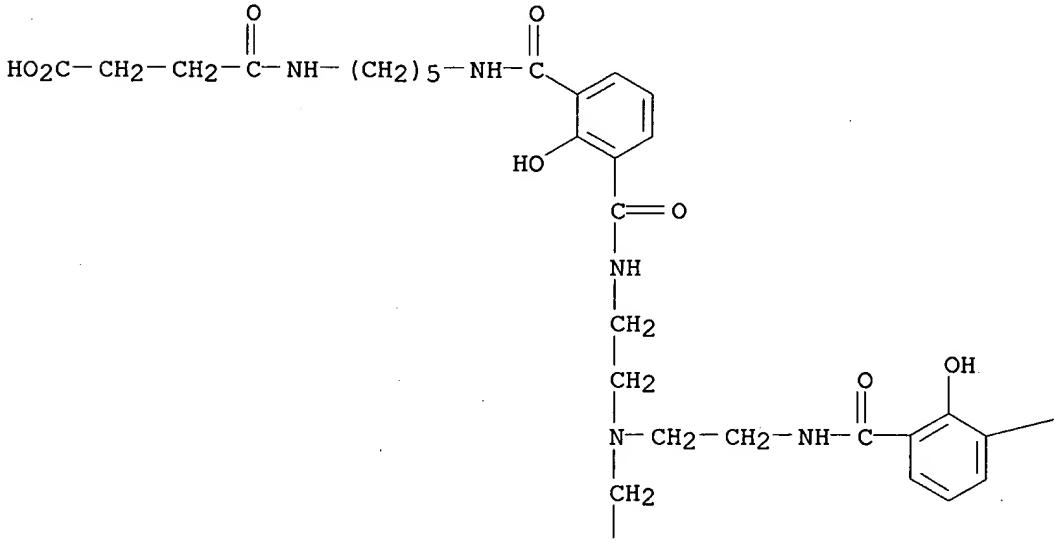

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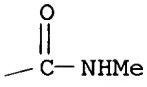

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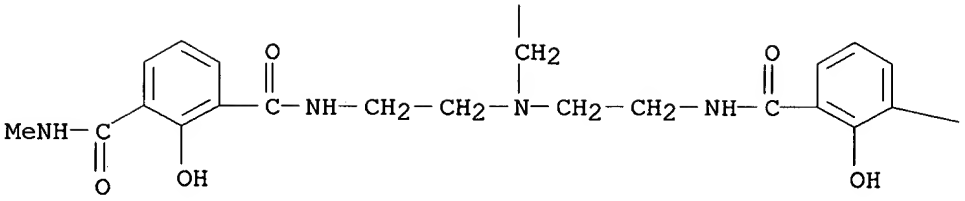

●2 HBr

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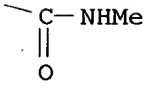

RN 288099-71-8 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'',N'''',N''''''-[1,2-ethanediylbis(nitrilodi-2,1-ethanediyl)]tetrakis[N'-(6-aminohexyl)-2-hydroxy- (9CI) (CA INDEX NAME)

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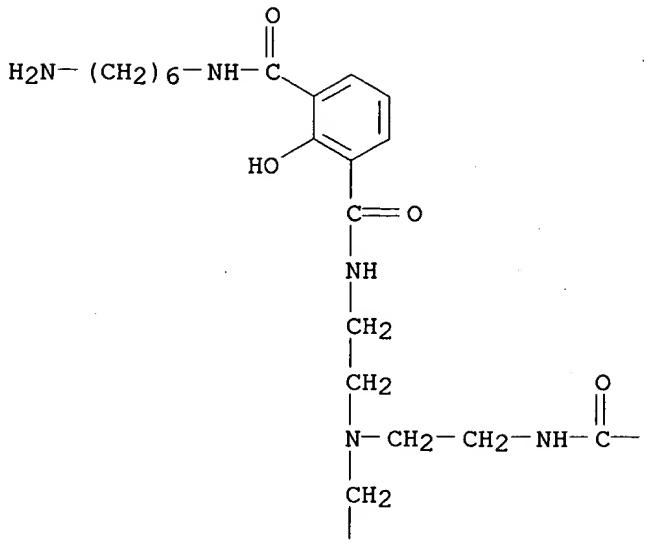

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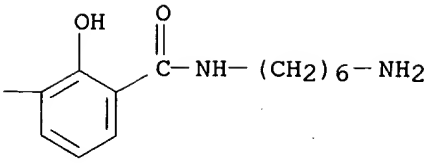

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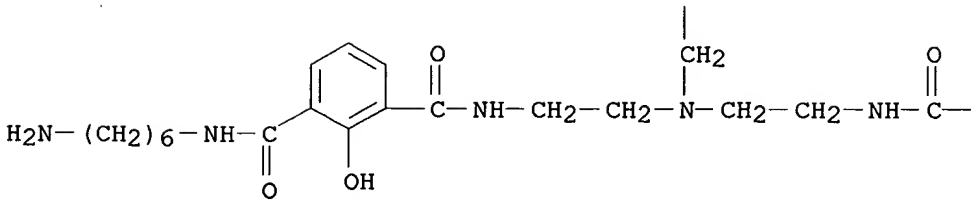

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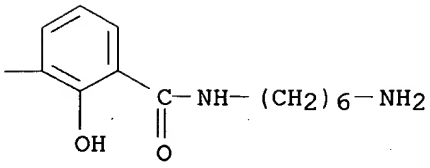

RN 288099-75-2 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'',N'''',N''''''-[1,3-propanediylbis(nitrilodi-2,1-ethanediyl)]tetrakis[2-hydroxy-N'-methyl-(9CI) (CA INDEX NAME)

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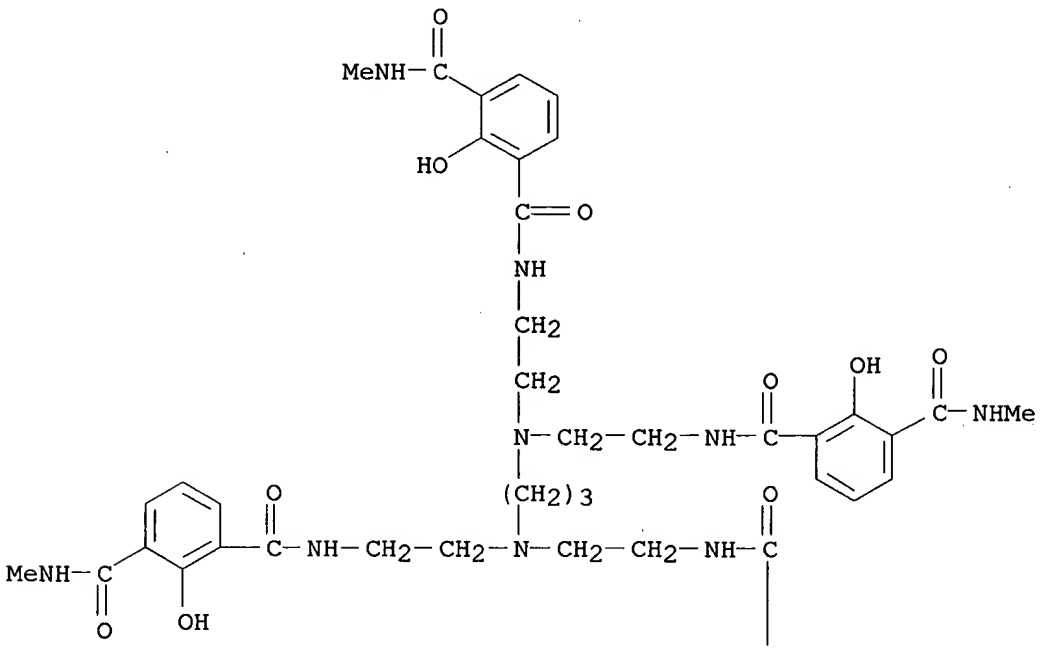

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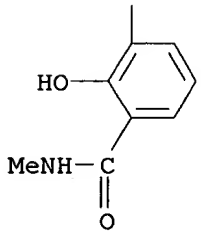

RN 288099-76-3 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'',N'''',N''''''-[1,4-butanediylbis(nitrilodi-2,1-ethanediyl)]tetrakis[2-hydroxy-N'-methyl- (9CI) (CA INDEX NAME)

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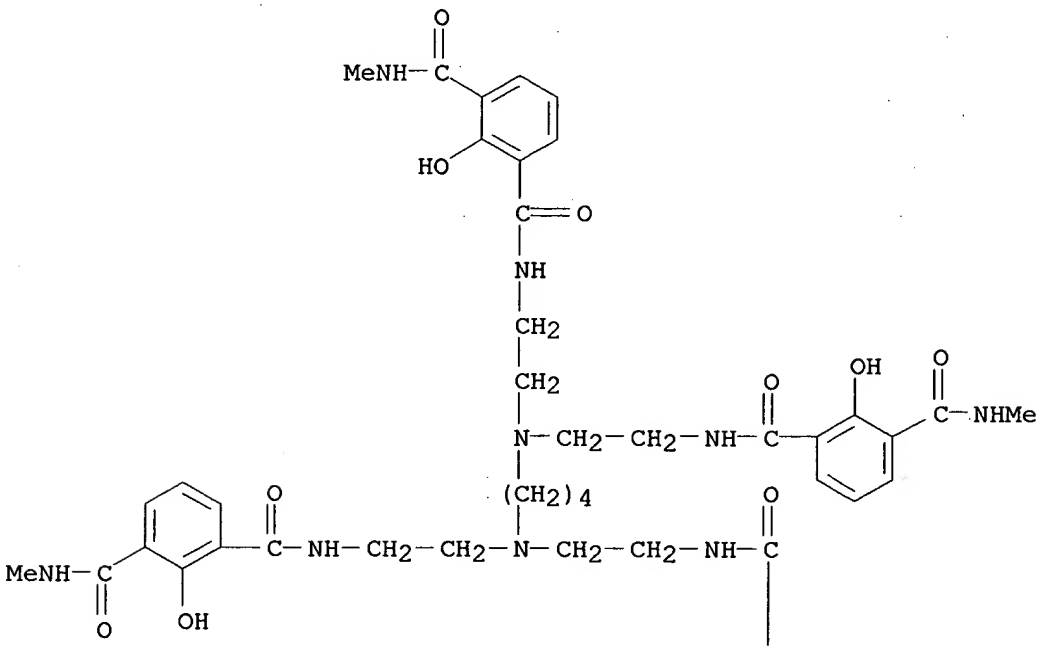

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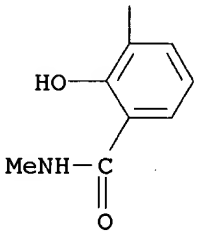

IT **288099-63-8DP**, complexes with europium, terbium, and lanthanum

288099-69-4DP, complexes with lanthanide ions
288099-71-8DP, complexes with lanthanide ions
RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. as luminescent marker)

RN 288099-63-8 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'',N'''',N''''''-[1,2-ethanediylbis(nitrilodi-2,1-ethanediyl)]tetrakis[2-hydroxy-N'-methyl- (9CI) (CA INDEX NAME)

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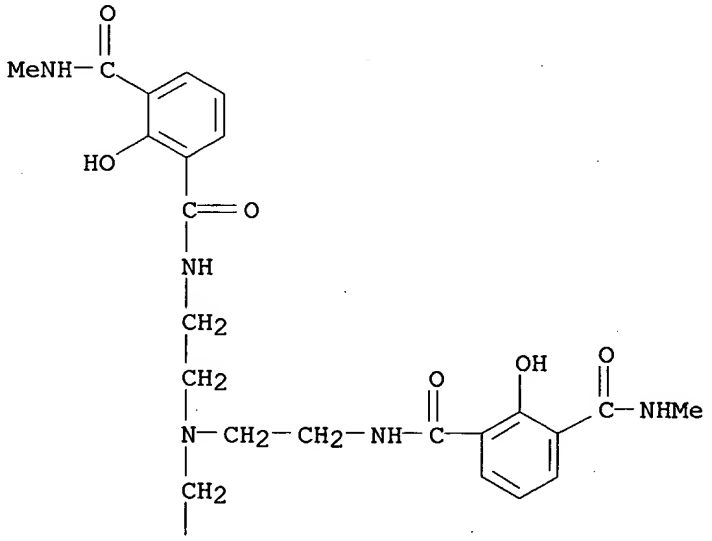

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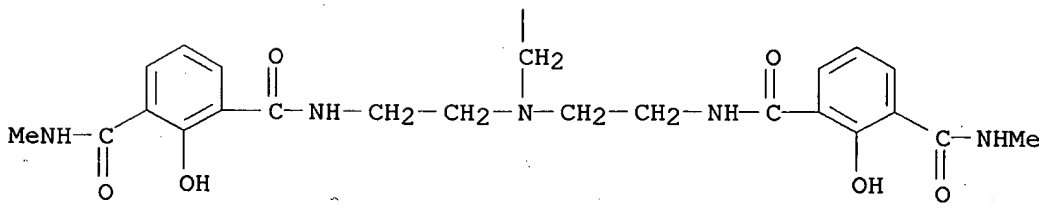

RN 288099-69-4 HCAPLUS
CN Butanoic acid, 4-[[5-[[3-[5,8-bis[2-[[2-hydroxy-3-[(methylamino)carbonyl]benzoyl]amino]ethyl]-12-[2-hydroxy-3-[(methylamino)carbonyl]phenyl]-1,12-dioxo-2,5,8,11-tetraazadodec-1-yl]-2-hydroxybenzoyl]amino]pentyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

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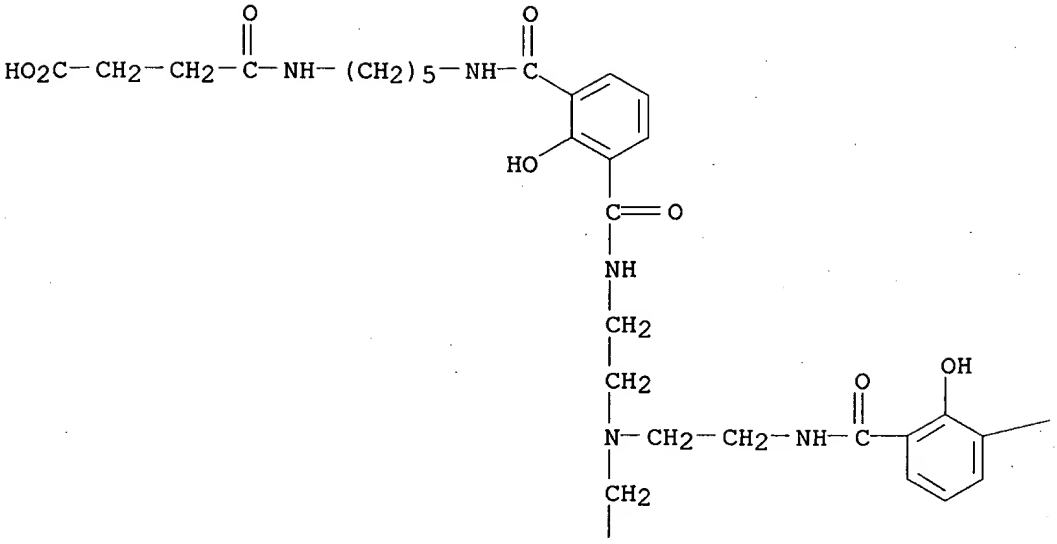

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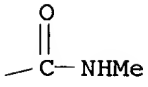

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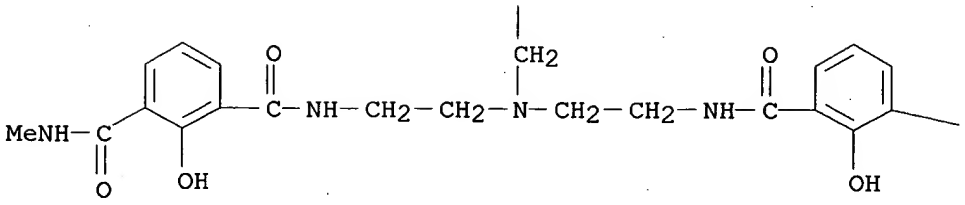

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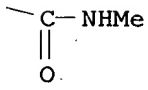

RN 288099-71-8 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'',N'''',N''''''-[1,2-ethanediylbis(nitrilodi-2,1-ethanediyl)]tetrakis[N'-(6-aminohexyl)-2-hydroxy- (9CI) (CA INDEX NAME)

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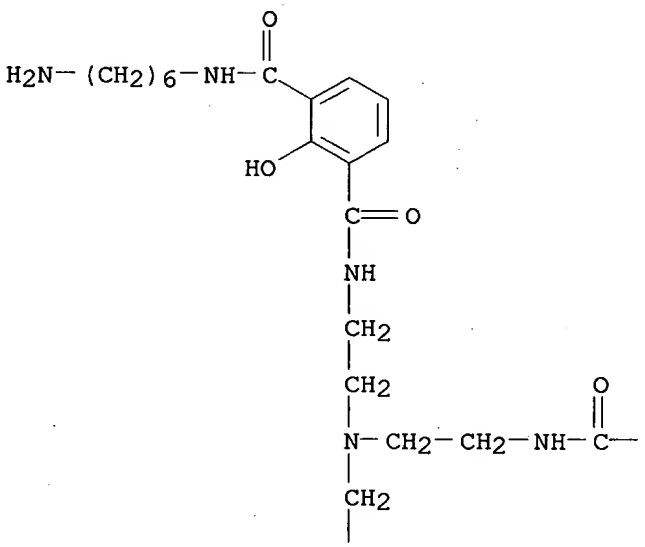

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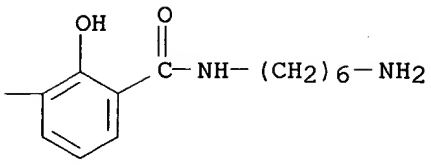

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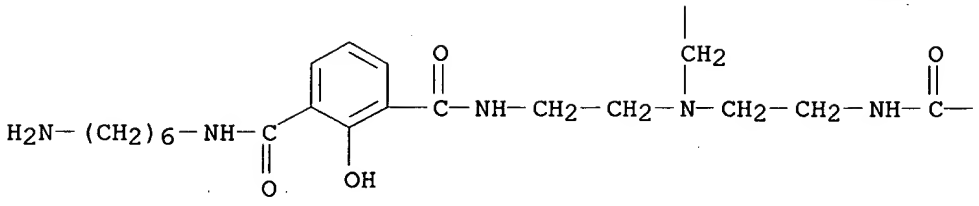

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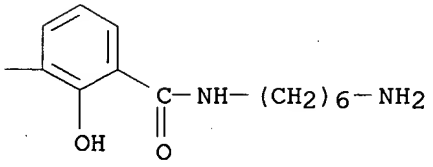

IT **288099-66-1DP**, lanthanide complexes and derivs. with/without carrier mols.
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. as luminescent markers)
RN 288099-66-1 HCAPLUS
CN 1,4,7,15,18,21,24,32,37,45,52,60-Dodecaazaheptacyclo[19.13.13.134,18.19,13

.126,30.139,43.154,58]tetrahexaconta-9,11,13(63),26,28,30(49),39,41,43(48)
,54,56,58(64)-dodecaene-8,14,26,31,38,44,53,59-octone,
48,49,63,64-tetrahydroxy- (9CI) (CA INDEX NAME)

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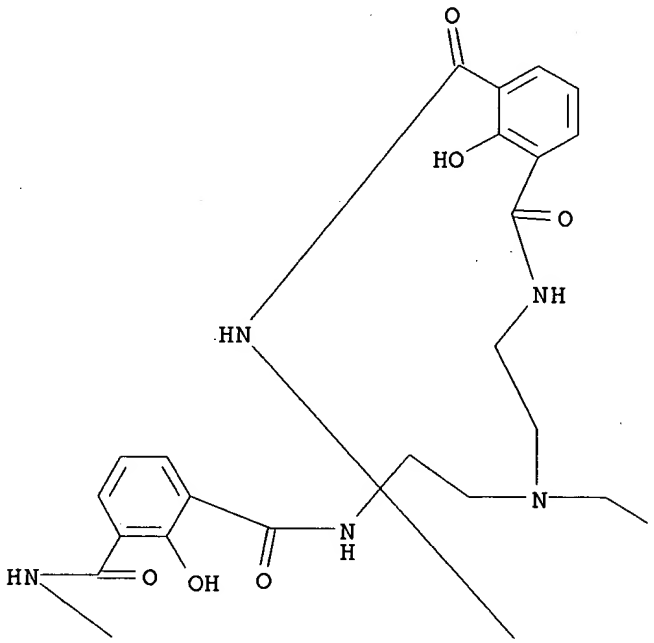

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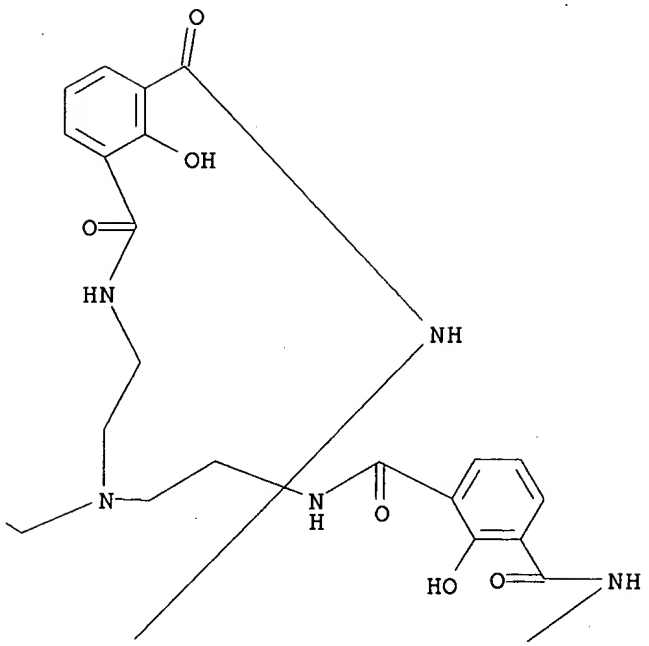

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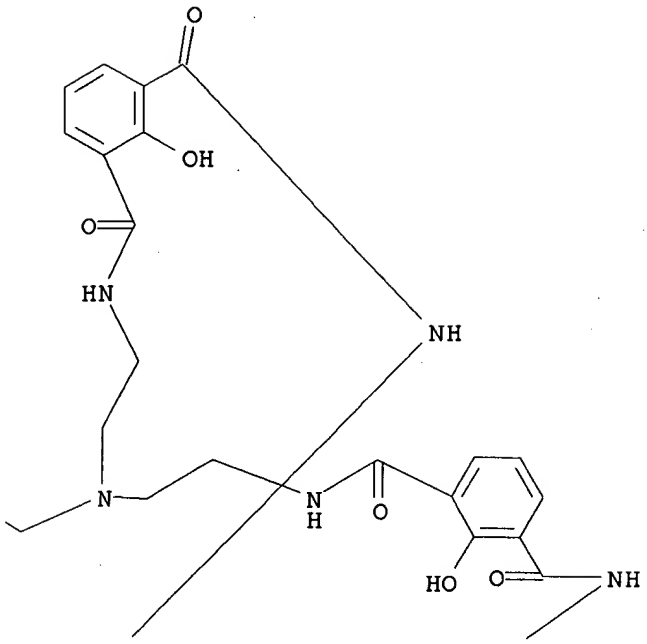

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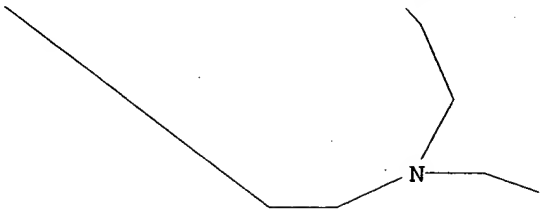

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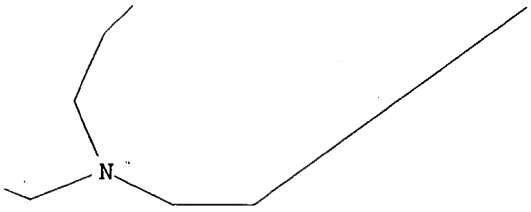

IT **288099-62-7P 288099-65-0P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn., luminescence, and complexation with lanthanide ions)
RN 288099-62-7 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'',N'''',N''''''-[1,2-ethanediylbis(nitrilodi-2,1-ethanediyl)]tetrakis[2-hydroxy-N'-methyl-, dihydrobromide (9CI) (CA

INDEX NAME)

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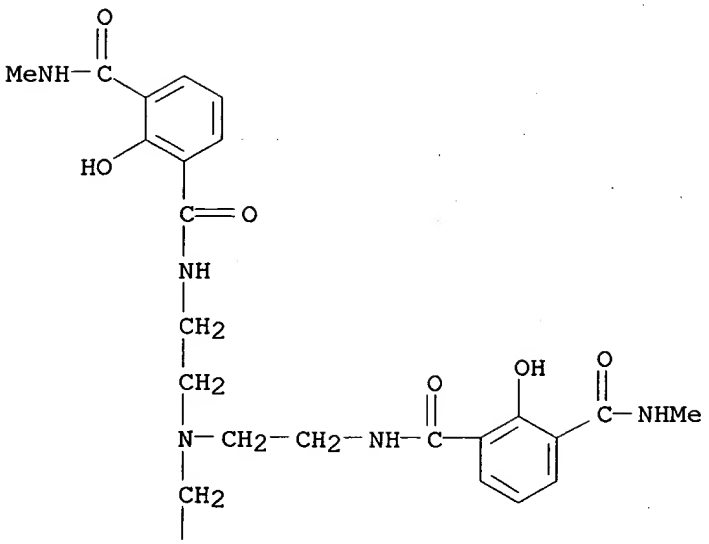

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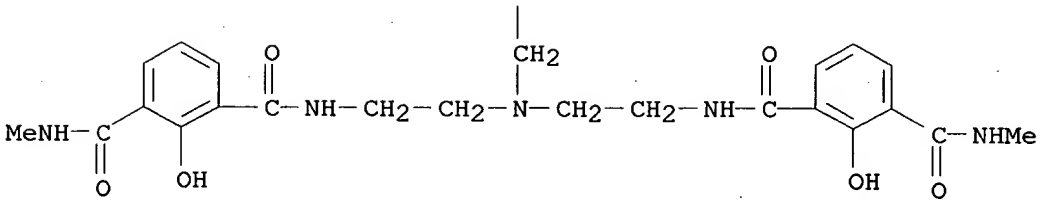

●2 HBr

RN 288099-65-0 HCAPLUS
CN 1,4,7,15,18,21,24,32,37,45,52,60-Dodecaazaheptacyclo[19.13.13.134,18.19,13.126,30.139,43.154,58]tetrahexaconta-9,11,13(63),26,28,30(49),39,41,43(48),54,56,58(64)-dodecaene-8,14,26,31,38,44,53,59-octone, 48,49,63,64-tetrahydroxy-, tetrahydrobromide (9CI) (CA INDEX NAME)

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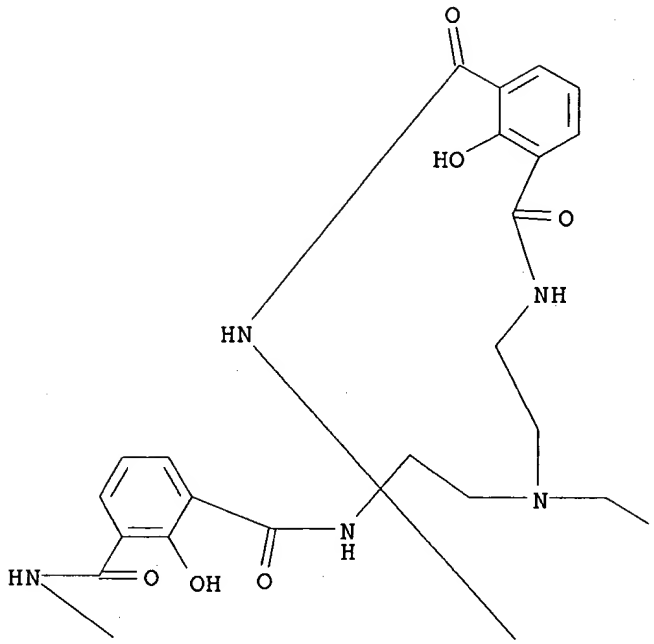

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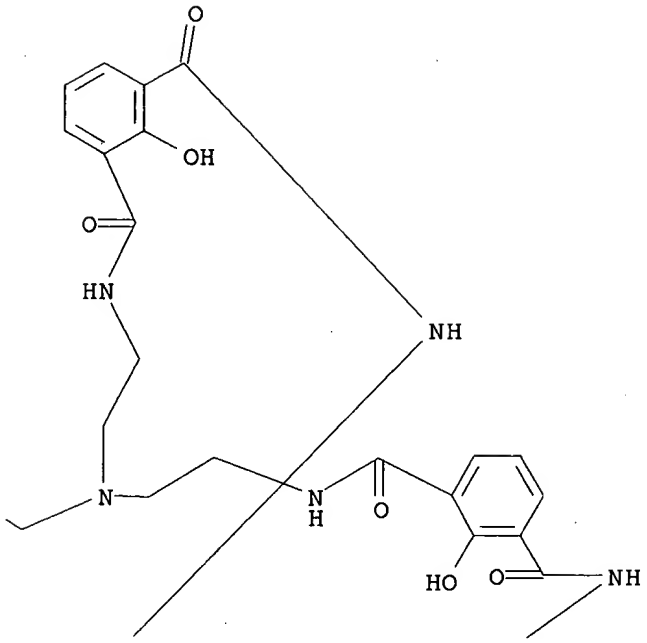

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●4 HBr

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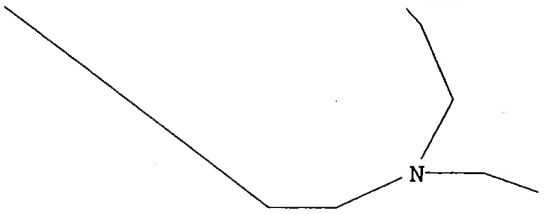

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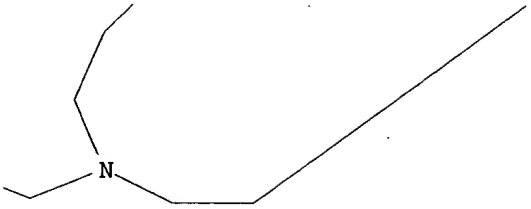

IT **288099-57-0P**
RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn., luminescence, and photophys. properties as luminescent marker)
RN 288099-57-0 HCAPLUS
CN Terbium(1+), bis[43,44-di(hydroxy-.kappa.O)-42-hydroxy-1,4,12,15,18,26,31,39-octaazapentacyclo[13.13.13.16,10.120,24.133,37]tetratetraconta-6,8,10(44),20,22,24(43),33,35,37(42)-nonaene-5,11,19,25,32,38-hexonato-.kappa.O5,.kappa.O19]- (9CI) (CA INDEX NAME)

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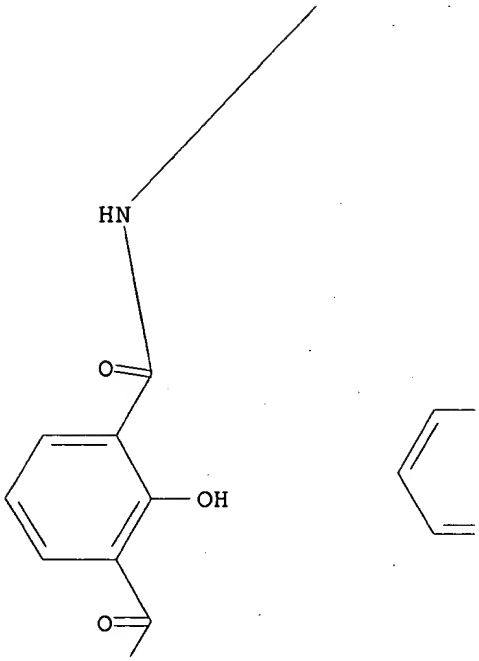

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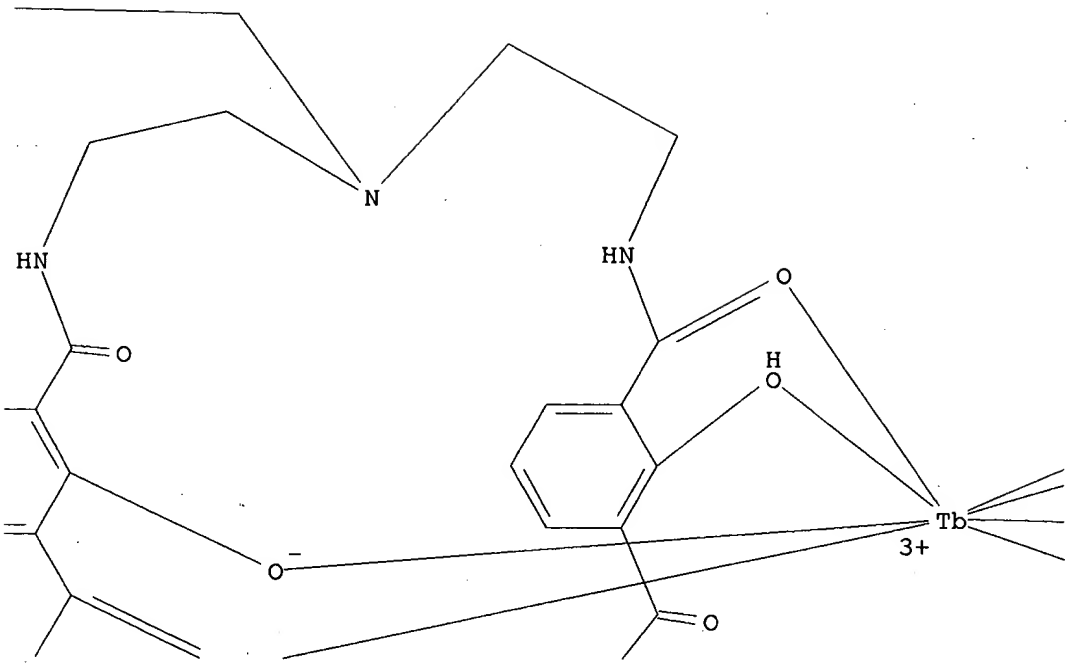

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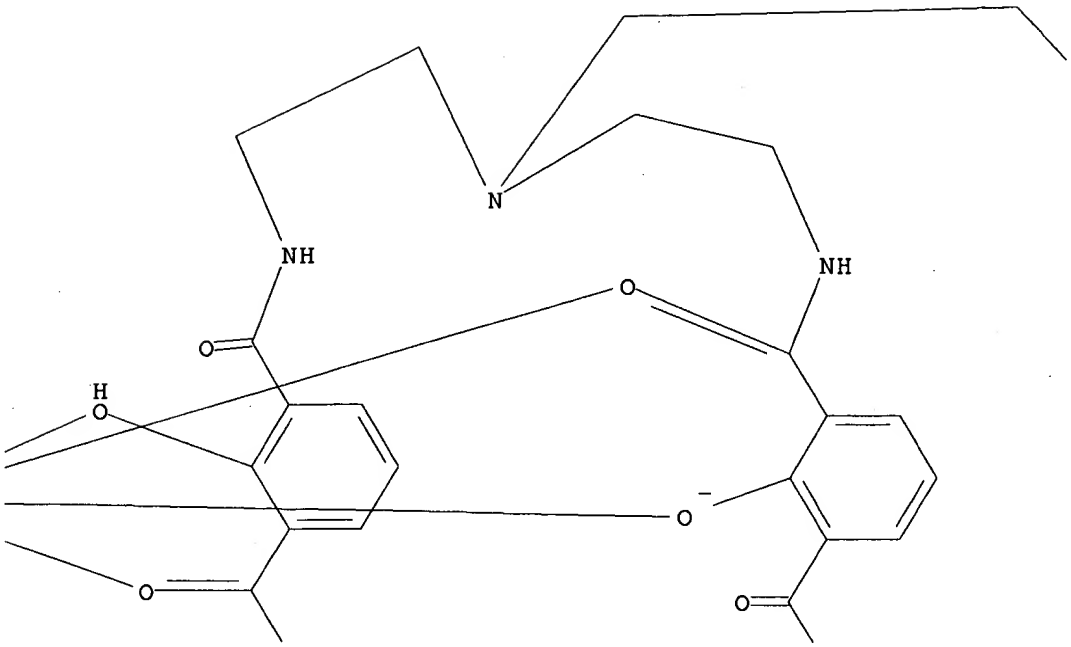

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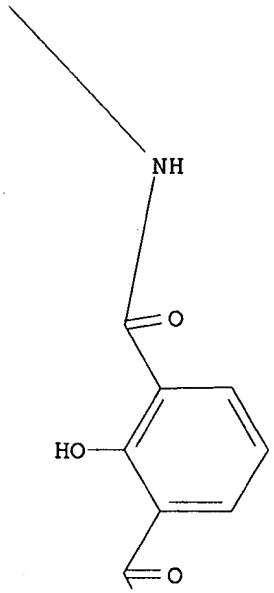

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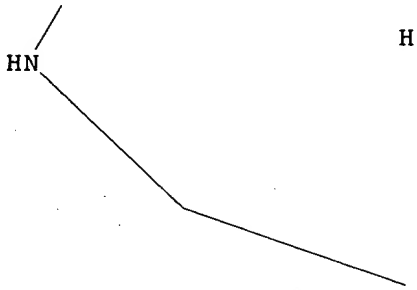

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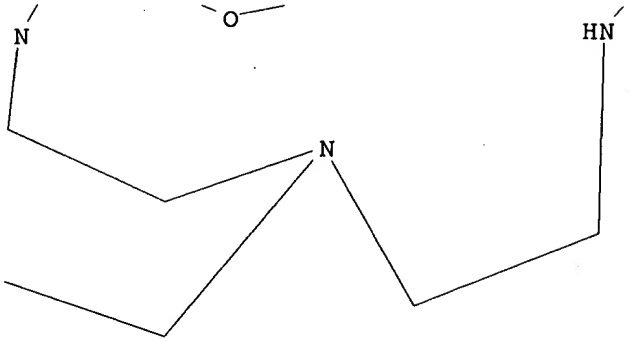

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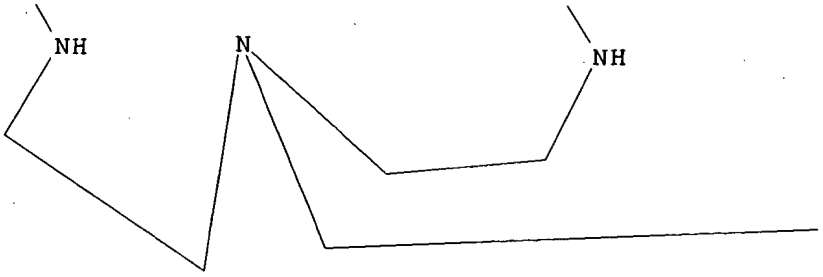

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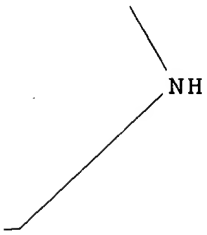
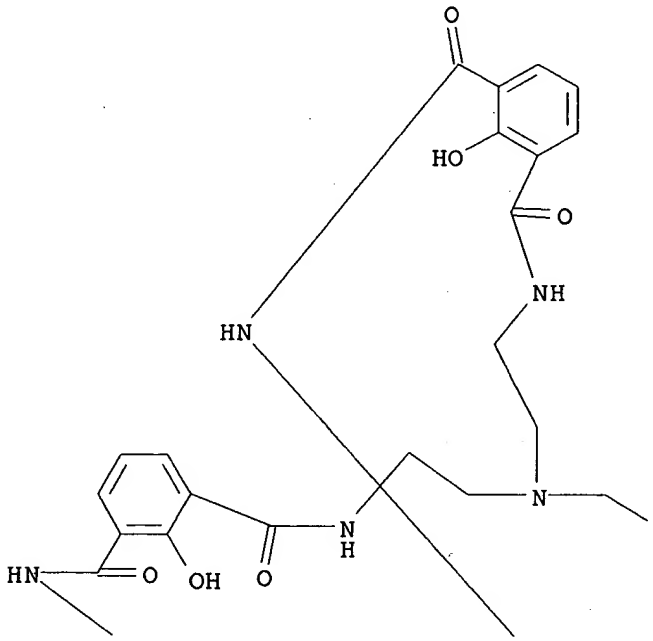


IT **288099-66-1DP**, terbium complex
RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn., luminescence, photophys. properties, and stability in DMSO or water as luminescent marker)

RN 288099-66-1 HCAPLUS

CN 1,4,7,15,18,21,24,32,37,45,52,60-Dodecaazaheptacyclo[19.13.13.134,18.19,13.126,30.139,43.154,58]tetrahexaconta-9,11,13(63),26,28,30(49),39,41,43(48),54,56,58(64)-dodecaene-8,14,26,31,38,44,53,59-octone, 48,49,63,64-tetrahydroxy- (9CI) (CA INDEX NAME)

PAGE 1-A



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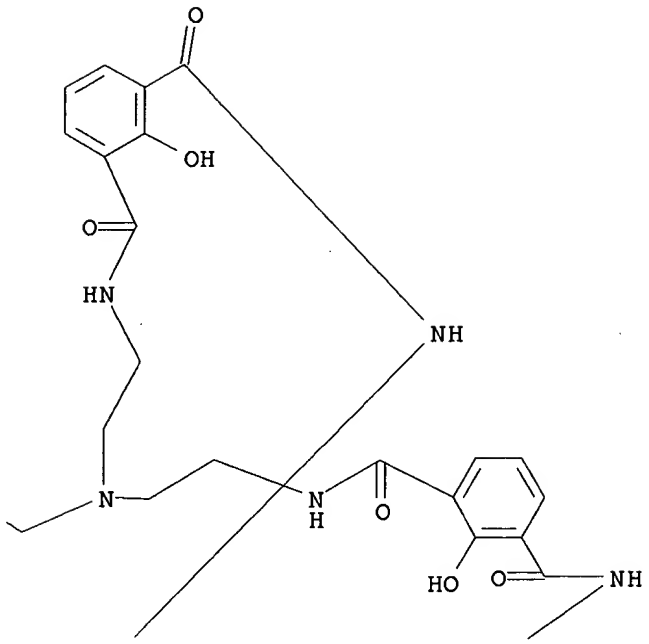

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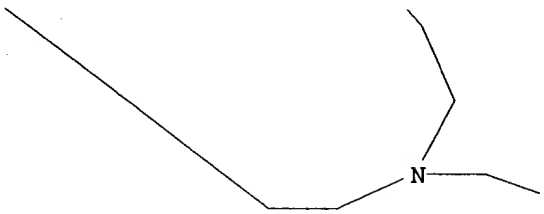

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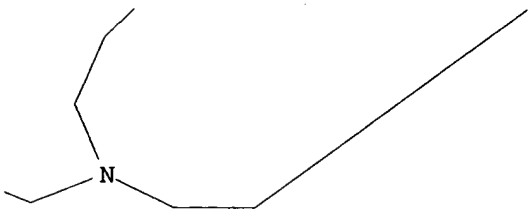

IT **288099-59-2P**
RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn., mol. structure, stability consts., luminescence, and photophys. properties as luminescent marker)
RN 288099-59-2 HCAPLUS

CN Terbium(1+), bis[43,44-di(hydroxy-.kappa.O)-42-hydroxy-1,4,12,15,18,26,31,39-octaazapentacyclo[13.13.13.16,10.120,24.133,37]tetratetraconta-6,8,10(44),20,22,24(43),33,35,37(42)-nonaene-5,11,19,25,32,38-hexonato-.kappa.O5,.kappa.O19]-, bromide, compd. with N,N-dimethylformamide (1:1), decahydrate (9CI) (CA INDEX NAME)

CM 1

CRN 288099-58-1
CMF C72 H82 Eu N16 O18 . Br
CCI CCS

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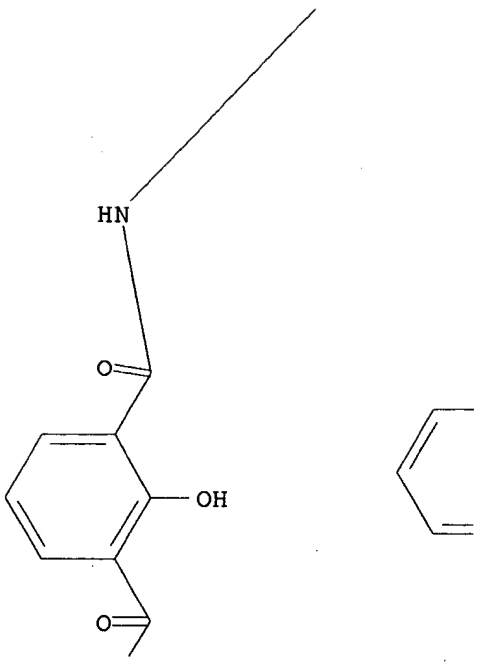
PAGE 1-C

PAGE 2-B



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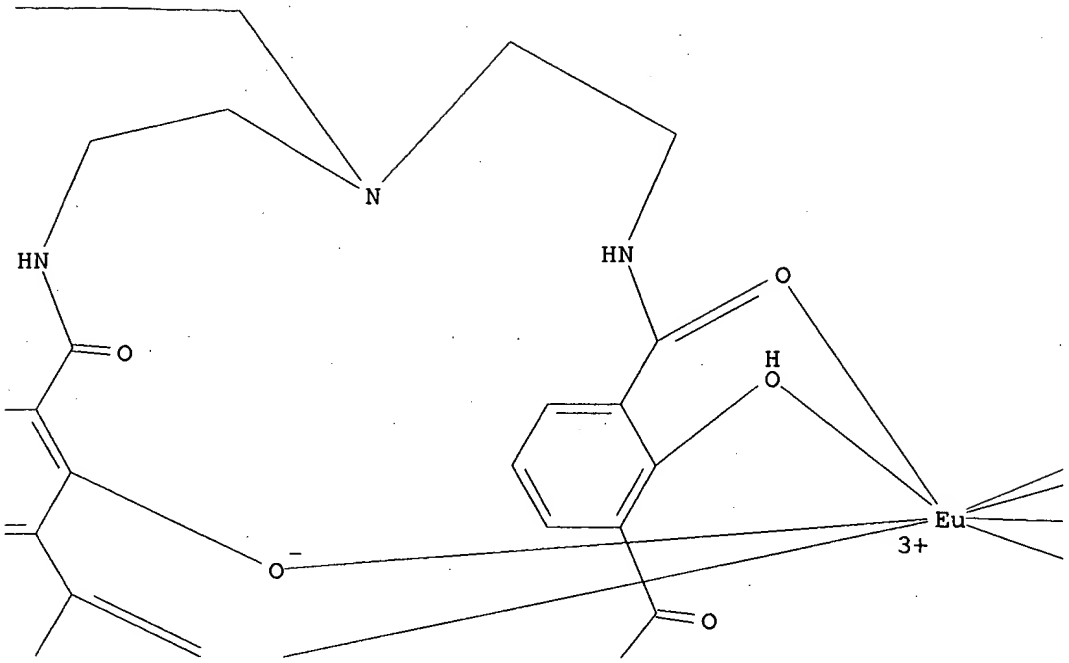

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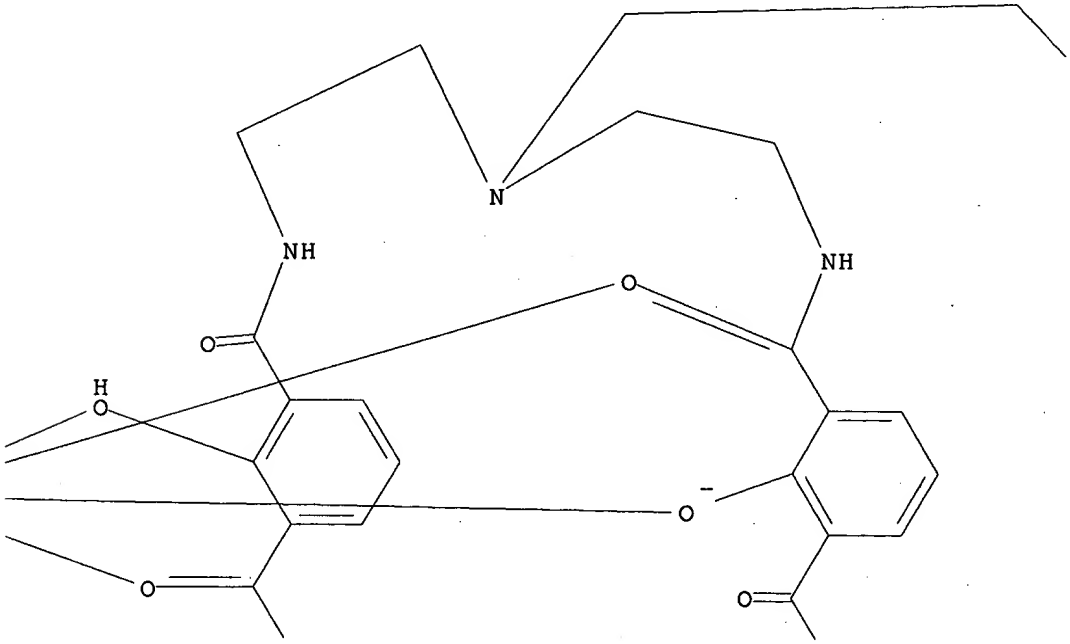

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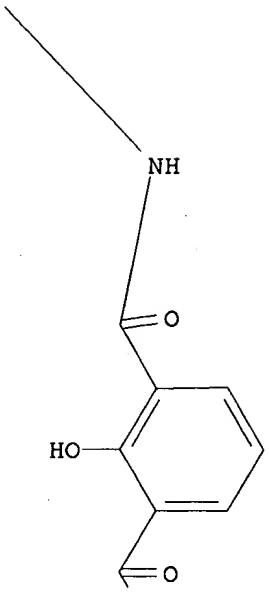

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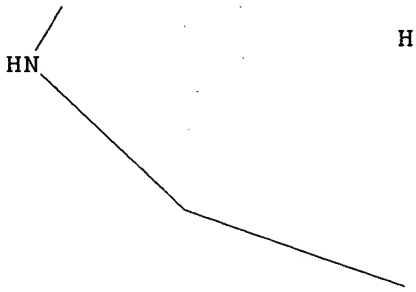
● Br^-

PAGE 3-B



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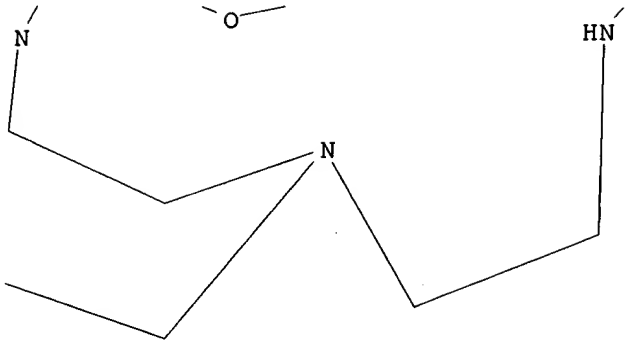

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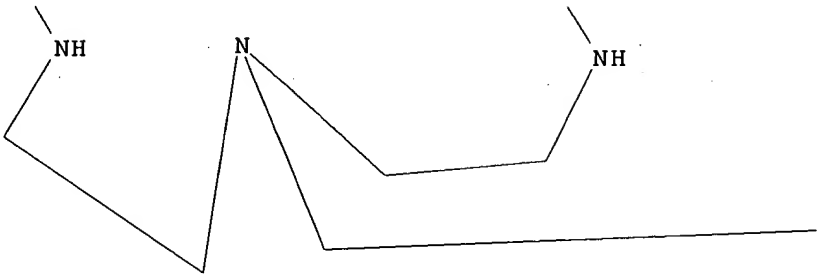

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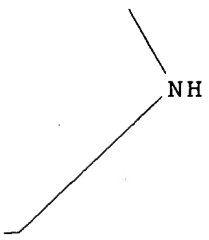
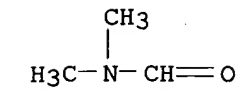


CM 2

CRN 68-12-2
CMF C3 H7 N O



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:580115 HCAPLUS
DOCUMENT NUMBER: 131:306351
TITLE: A Novel Salicylate-Based Macrobicycle with a "Split Personality"
AUTHOR(S): Cohen, Seth M.; Petoud, Stephane; Raymond, Kenneth N.
CORPORATE SOURCE: Department of Chemistry, University of California, Berkeley, CA, 94720, USA
SOURCE: Inorganic Chemistry (1999), 38(20), 4522-4529
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

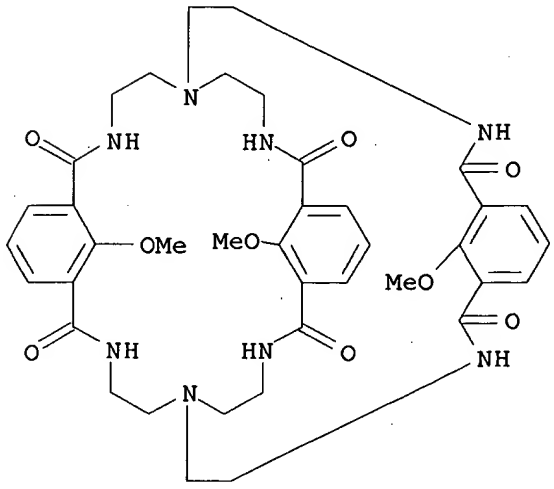
AB Two new ligands (tripodal TRENIAM and macrobicyclic TRENSAM) which use 2-hydroxyisophthalic acid as a salicylato-type of binding group were prepd, and their coordination chem. was studied. The structures of several metal complexes were detd. in both soln. and the solid state. The Fe and Ga complexes of TRENIAM are isostructural and crystallize in the triclinic space group P.hivin.1, with Z = 4. Lattice parameters for Fe[TRENIAM] are a 12.0203(4), b 12.6996(4), c 24.6435(8) .ANG., .alpha. 83.146(1), .beta. 88.531(1), .gamma. 85.282(1).degree.. Lattice parameters for Ga[TRENIAM] are a 11.9780(2), b 12.6417(3), c 24.5404(6) .ANG., .alpha. 83.324(1), .beta. 88.488(1), .gamma. 85.038(1).degree.. The metal cations are bound by three phenolic oxygens and three carbonyl oxygens in a ligand structure analogous to that of salicylamide. The Fe and Ga complexes of macrobicyclic TRENSAM are essentially isosteric and crystallize in the monoclinic space group P21/n, with Z = 4. For Fe[macrobicyclic TRENSAM]+: a 10.7156(2), b 23.10490(10), c 19.8373(3) .ANG., .beta. 98.829(1).degree.. For Ga[macrobicyclic TRENSAM]+: a 11.1144(2), b 22.8382(4), c 19.4525(4) .ANG., .beta. 99.247(1).degree.. The metal complexes of macrobicyclic TRENSAM impose an unusual conformational distortion on the macrobicycle, breaking the C2 symmetry axis of the parent ligand. This results in a macrocyclic complex with two acyclic analogs, TRENSAM and TRENIAM, giving the cryptate a split personality with structural features of both acyclic ligands. 1H NMR shows that the metal complexes of macrobicyclic TRENSAM are kinetically inert and retain an asym. structure in soln. Cyclic voltammetry expts. show that the ferrous complexes are strongly stabilized by the macrocyclic structure.

IT **247039-38-9P 247039-39-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(for prepn. of transition metal macrocyclic hydroxyisophthalic acid deriv. complexes)

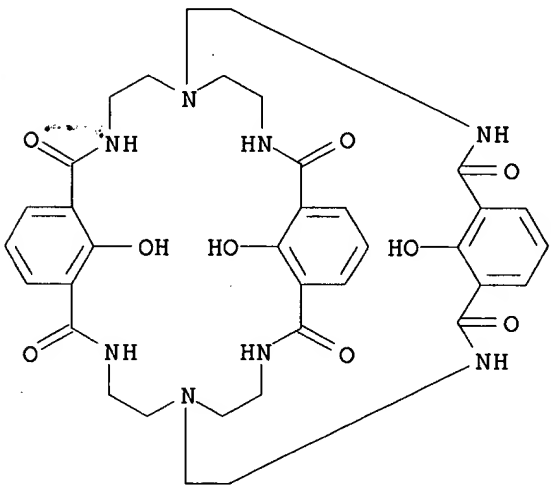
RN 247039-38-9 HCAPLUS

CN 1,4,12,15,18,26,31,39-Octaazapentacyclo[13.13.13.16,10.120,24.133,37]tetra tetraconta-6,8,10(44),20,22,24(43),33,35,37(42)-nonaene-5,11,19,25,32,38-hexone, 42,43,44-trimethoxy- (9CI) (CA INDEX NAME)



RN 247039-39-0 HCAPLUS

CN 1,4,12,15,18,26,31,39-Octaazapentacyclo[13.13.13.16,10.120,24.133,37]tetra tetraconta-6,8,10(44),20,22,24(43),33,35,37(42)-nonaene-5,11,19,25,32,38-hexone, 42,43,44-trihydroxy-, dihydrobromide (9CI) (CA INDEX NAME)



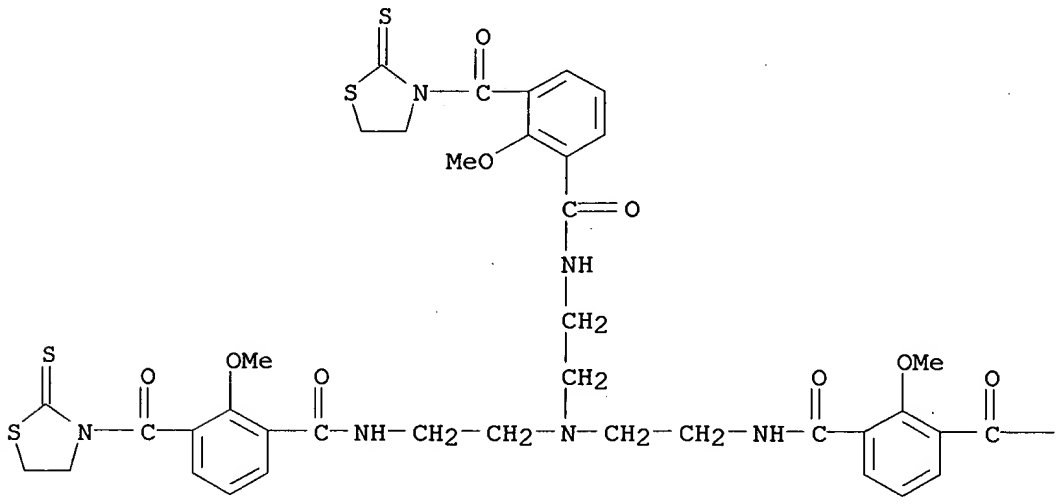
●2 HBr

IT **247039-31-2P 247039-32-3P 247039-33-4P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for prepn. of transition metal tripodal hydroxyisophthalic acid deriv. complexes)

RN 247039-31-2 HCAPLUS
CN Benzamide, N,N',N''-(nitrilotri-2,1-ethanediyl)tris[2-methoxy-3-[(2-thioxo-3-thiazolidinyl)carbonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



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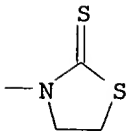
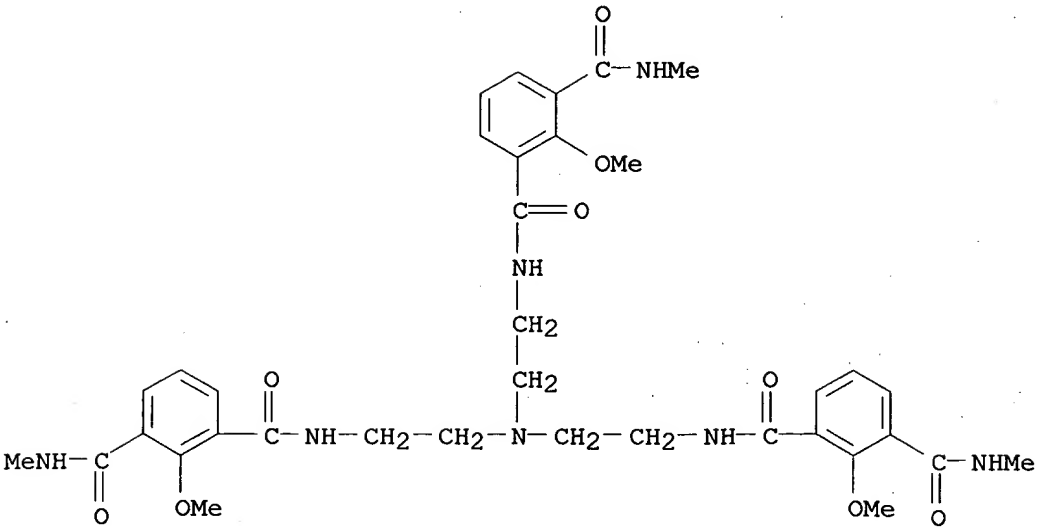
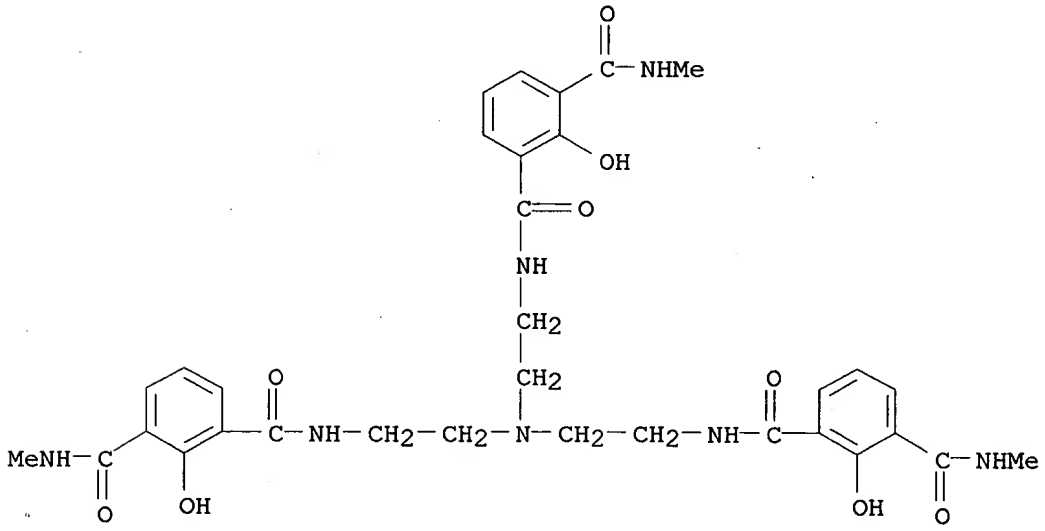


RN 247039-32-3 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'',N''''-(nitrilotri-2,1-ethanediyl)tris[2-methoxy-N'-methyl- (9CI) (CA INDEX NAME)



RN 247039-33-4 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'',N''''-(nitrilotri-2,1-ethanediyl)tris[2-hydroxy-N'-methyl-, monohydrobromide (9CI) (CA INDEX NAME)

PAGE 1-A



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● HBr

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:681250 HCAPLUS
DOCUMENT NUMBER: 127:331474
TITLE: Synthesis of macrocyclic polyhydroxy tetralactams derived from L-tartaric acid and .beta.-hydroxyglutaric acid
AUTHOR(S): Arnaud, Nathalie; Picard, Claude; Cazaux, Louis; Tisnes, Pierre
CORPORATE SOURCE: Synthese et Physicochimie Organique Unite associee au CNRS ESA 5068, Universite Paul Sabatier, Toulouse, 31062, Fr.
SOURCE: Tetrahedron (1997), 53(40), 13757-13768
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

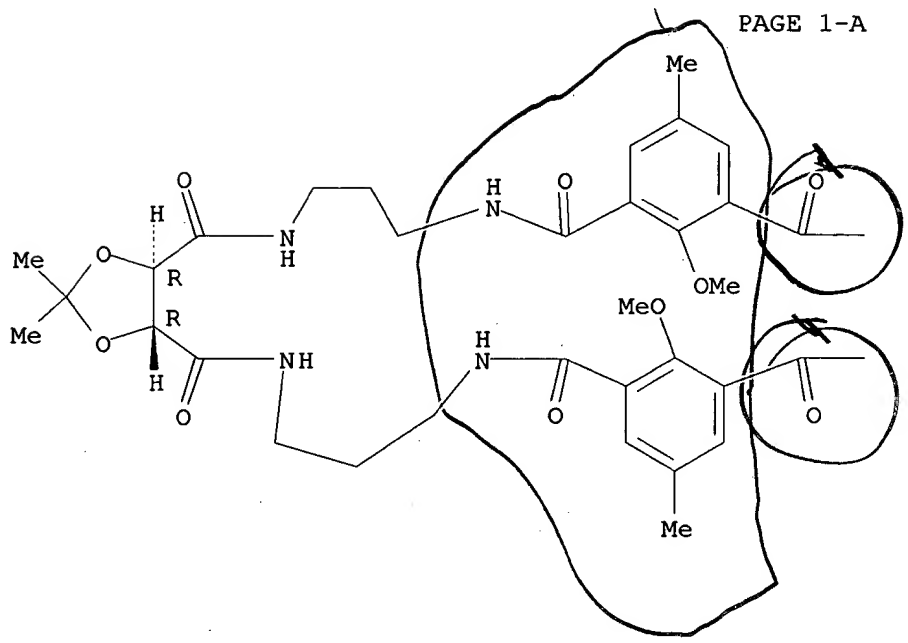
AB The synthesis of new 16-, 18-, 19- or 20-membered secondary tetralactams with L-tartaric acid or .beta.-hydroxyglutaric acid moieties is investigated. The stepwise synthesis with an intermediate diamide diamine provides overall good yields (30-55%) compared with other processes using an intermediate diamide diacid or direct macrocyclization. This synthetic pathway leads to sym. or unsym. polyhydroxytetralactams with variable hydroxyl group no. Use of mild acylating agents avoids the protection-deprotection of hydroxyl groups.

IT **197906-47-1P 197906-49-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of macrocyclic tetralactams derived from L-tartaric or .beta.-hydroxyglutaric acid)

RN 197906-47-1 HCAPLUS
CN 11,15:33,37-Dimethenobis[1,3]dioxolo[4,5-g:4',5'-b1][1,5,10,14,22,26,31,35]octaazacyclodotetracontine-4,10,16,22,26,32,38,44(5H,17H,27H,39H)-octone, 3a,6,7,8,9,18,19,20,21,22a,25a,28,29,30,31,40,41,42,43,44a-eicosahydro-45,46-dimethoxy-2,2,13,24,24,35-hexamethyl-, [3aR-(3aR*,22aR*,25aR*,44aR*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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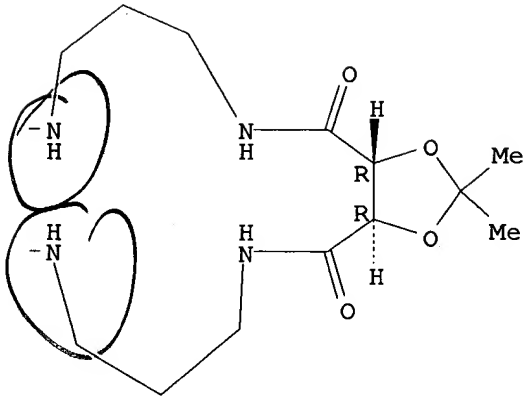
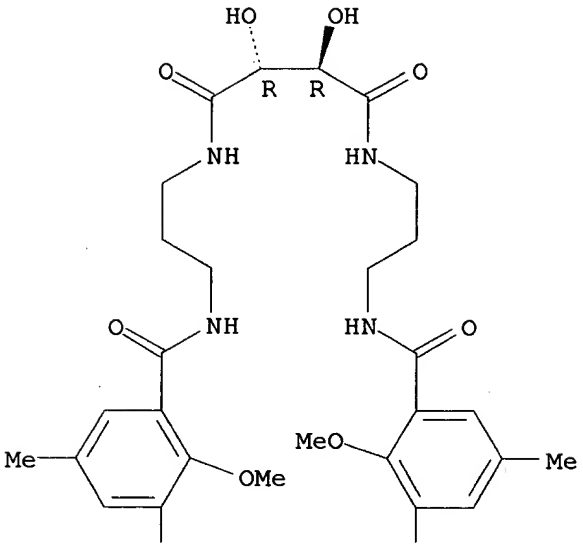


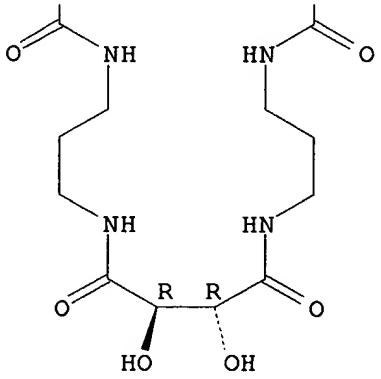
RN 197906-49-3 HCAPLUS
CN 3,7,12,16,24,28,33,37-Octaazatricyclo[37.3.1.118,22]tetratetraconta-1(43),18,20,22(44),39,41-hexaene-2,8,11,17,23,29,32,38-octone, 9,10,30,31-tetrahydroxy-43,44-dimethoxy-20,41-dimethyl-, [9R-(9R*,10R*,30R*,31R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



L16 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:404021 HCAPLUS
DOCUMENT NUMBER: 127:135782
TITLE: Synthesis of novel C2 symmetric receptors containing a diaza-crown macrocycle
AUTHOR(S): Kim, Tae Woo; Ryu, Gean Ha; Chung, Doo Soo; Hong, Jong-In
CORPORATE SOURCE: Dep. Chem., Seoul National Univ., Seoul, 151-742, S. Korea
SOURCE: Bulletin of the Korean Chemical Society (1997), 18(5), 558-561

CODEN: BKCSDE; ISSN: 0253-2964
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Diaza-crown macrocycles were prepd. and complexation data with picrates are provided.

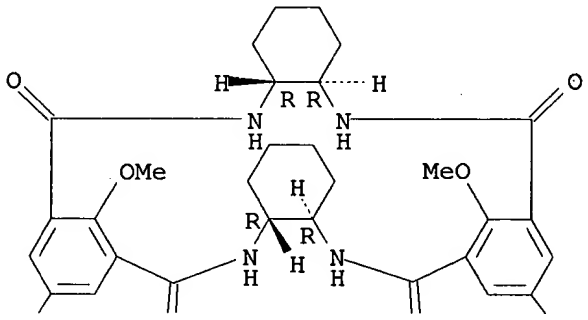
IT **192936-74-6DP**, cesium and potassium complexes **192936-79-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and complexation of diaza-crown macrocycles with alkali and ammonium picrates)

RN 192936-74-6 HCAPLUS

CN 29,38-(Ethanoxyethanoxyethano)-9,22-(methaniminoethanoxyethanoxyethanimino methano)-7,11:20,24-dimethenodibenzo[b,m][1,4,12,15]tetraazacyclodocosine-6,12,19,25-tetrone, 1,2,3,4,4a,5,13,13a,14,15,16,17,17a,18,26,26a-hexadecahydro-27,40-dimethoxy-, [4aR-(4aR*,13aR*,17aR*,26aR*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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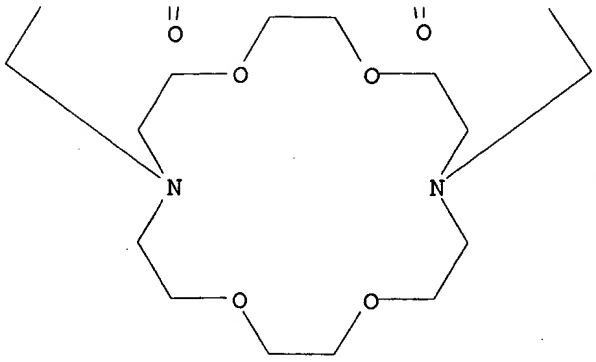

RN 192936-79-1 HCAPLUS
CN 29,38-(Ethanoxyethanoxyethano)-9,22-(methaniminoethanoxyethanoxyethanimino methano)-7,11:20,24-dimethenodibenzo[b,m][1,4,12,15]tetraazacyclodocosine-6,12,19,25-tetrone, 1,2,3,4,4a,5,13,13a,14,15,16,17,17a,18,26,26a-hexadecahydro-27,40-dimethoxy-, [4aR-(4aR*,13aR*,17aR*,26aR*)]-, compd. with 2,4,6-trinitrophenol ammonium salt (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 192936-74-6
CMF C44 H62 N6 O10

Absolute stereochemistry.

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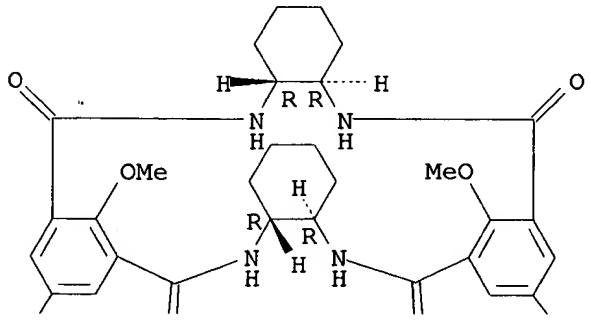

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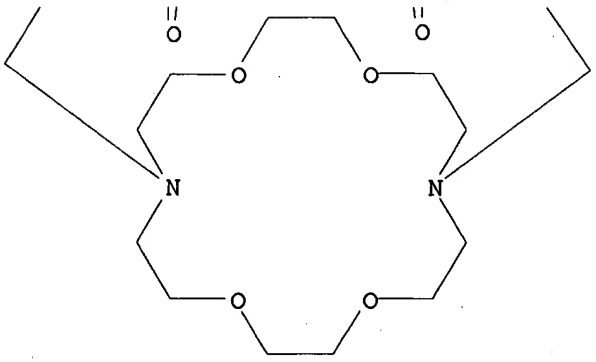
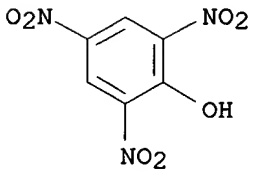


CM 2

CRN 131-74-8
CMF C6 H3 N3 O7 . H3 N

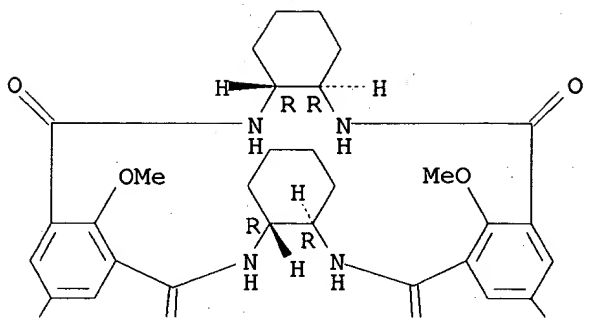


● NH_3

IT **192936-74-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and complexation of diaza-crown macrocycles with alkali and ammonium picrates)
RN 192936-74-6 HCAPLUS
CN 29,38-(Ethanoxyethanoxyethano)-9,22-(methaniminoethanoxyethanoxyethanimino methano)-7,11:20,24-dimethenodibenzo[b,m][1,4,12,15]tetraazacyclodocosine-6,12,19,25-tetrone, 1,2,3,4,4a,5,13,13a,14,15,16,17,17a,18,26,26a-hexadecahydro-27,40-dimethoxy-, [4aR-(4aR*,13aR*,17aR*,26aR*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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